WEST Search History

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DATE: Friday, August 20, 2004

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☐	L2	L1 same database	136
☐	L1	sequence same search same (iterative or sequential)	949

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 NEWS  1           Web Page URLs for STN Seminar Schedule - N. America
 NEWS  2           "Ask CAS" for self-help around the clock
 NEWS  3  May 12   EXTEND option available in structure searching
 NEWS  4  May 12   Polymer links for the POLYLINK command completed in REGISTRY
 NEWS  5  May 27   New UPM (Update Code Maximum) field for more efficient patent
                   SDIs in CAplus
 NEWS  6  May 27   CAplus super roles and document types searchable in REGISTRY
 NEWS  7  Jun 28   Additional enzyme-catalyzed reactions added to CASREACT
 NEWS  8  Jun 28   ANTE, AQUALINE, BIOENG, CIVILENG, ENVIROENG, MECHENG,
                   and WATER from CSA now available on STN(R)
 NEWS  9  Jul 12   BEILSTEIN enhanced with new display and select options,
                   resulting in a closer connection to BABS
 NEWS 10  Jul 30   BEILSTEIN on STN workshop to be held August 24 in conjunction
                   with the 228th ACS National Meeting
 NEWS 11  AUG 02   IFIPAT/IFIUDB/IFICDB reloaded with new search and display
                   fields
 NEWS 12  AUG 02   CAplus and CA patent records enhanced with European and Japan
                   Patent Office Classifications
 NEWS 13  AUG 02   STN User Update to be held August 22 in conjunction with the
                   228th ACS National Meeting
 NEWS 14  AUG 02   The Analysis Edition of STN Express with Discover!
                   (Version 7.01 for Windows) now available
 NEWS 15  AUG 04   Pricing for the Save Answers for SciFinder Wizard within
                   STN Express with Discover! will change September 1, 2004

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               MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP),
               AND CURRENT DISCOVER FILE IS DATED 11 AUGUST 2004
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FILE 'HOME' ENTERED AT 15:39:31 ON 20 AUG 2004

=> file .pub
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FILE 'MEDLINE' ENTERED AT 15:39:40 ON 20 AUG 2004
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FILE 'BIOSIS' ENTERED AT 15:39:40 ON 20 AUG 2004
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=> e toldo l/au
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E3          18 --> TOLDO L/AU
E4           1     TOLDO L I/AU
E5           1     TOLDO L I G/AU
E6           1     TOLDO LUCA/AU
E7          16     TOLDO M/AU
E8           1     TOLDO M A/AU
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E11          4     TOLDO S SOLINAS/AU
E12          2     TOLDO SABINA SOLINAS/AU

=> s e3-6
L1          21 ("TOLDO L"/AU OR "TOLDO L I"/AU OR "TOLDO L I G"/AU OR "TOLDO
               LUCA"/AU)

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DUPLICATE PREFERENCE IS 'MEDLINE, BIOSIS'
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PROCESSING COMPLETED FOR L1
L2          18 DUPLICATE REMOVE L1 (3 DUPLICATES REMOVED)

=> d 1-18 bib ab

L2   ANSWER 1 OF 18     MEDLINE on STN
Full Text
AN   2004162614     IN-PROCESS
DN   PubMed ID: 15057406
TI   [Toxicoproteomics: first experiences in a BMBF-study].
     Toxikoproteomics: Erste Erfahrungen in einer BMBF-Studie.
AU   Kroger Michaela; Hellmann Jurgen; Toldo Luca; Gluckmann Matthias; von
     Eiff Bettina; Fella Kerstin; Kramer Peter-Jurgen
CS   Institut fur Toxikologie, Merck KGaA, D-Darmstadt..
     michaela.kroeger@merck.com
SO   ALTEX : Alternativen zu Tierexperimenten, (2004) 21 Suppl 3 28-40.
     Journal code: 100953980. ISSN: 0946-7785.
CY   Germany: Germany, Federal Republic of
DT   Journal; Article; (JOURNAL ARTICLE)
LA   German
FS   IN-PROCESS; NONINDEXED; Priority Journals
ED   Entered STN: 20040402
     Last Updated on STN: 20040505
AB   The rapid development of molecular toxicology is providing innovative
     approaches to an improved investigation and recognition of toxic
     substances.  Proteome analysis offers, with 2DE/MS (two-dimensional gel
     electrophoresis and mass spectrometry) and SELDI (surface enhanced laser
     desorption/ionisation), a promising discipline to classify molecular
     changes caused by toxic exposure.  The Rat Liver Foci Bioassay (RLFB) is a
     detailed, well-described model for the investigation of liver
     carcinogenesis induced by chemical substances.  Based on this model, we
     examined whether proteomic methods of molecular toxicology can be used for
     the early recognition of toxic and/or carcinogenic characteristics of
     toxic substances.  In addition, identification and subsequent
     prevalidation of new hepatocellular biomarkers was performed, enabling
     better prediction of toxic and/or carcinogenic effects.  This could lead
```

to a more meaningful RLFB and thus to an improved risk assessment of chemicals. 2DE analysis in this study showed that deregulated proteins are assigned to mainly anabolic and catabolic metabolism pathways in the cell. Beyond this, individual proteins were identified which play a key role in the carcinogenic process. A comparison of the differentially expressed proteins in tissue from tumour-bearing animals and tissue derived from the start of the study revealed that protein expression changes (biomarkers) were already detectable shortly after exposure. In addition, analysis by SELDI clearly showed several differentially expressed proteins and/or derived masses. The spectra represented specific differences in tissues, which could be assigned to the same histopathological endpoints. With bioinformatics analysis it was possible to identify individual discriminating mass peaks, which were indicative of tumour formation. Group specific changes can be illustrated and/or represented in more detail with further cluster analysis methods. These results give hope for an improved prediction of hepatotoxicity and carcinogenicity by means of protein markers, which could in the future lead to a shortening of carcinogenicity studies and to a reduction in the use of experimental animals.

L2 ANSWER 2 OF 18 BIOSIS COPYRIGHT 2004 BIOLOGICAL ABSTRACTS INC. on STN
Full Text
AN 2003:307420 BIOSIS
DN PREV200300307420
TI Biomarker identification in toxicology by SELDI.
AU Knapp, U. [Reprint Author]; Fella, K. [Reprint Author]; von Eiff, B. [Reprint Author]; **Toldo, L.**; Hellmann, J. [Reprint Author]; Kroeger, M. [Reprint Author]
CS Merck KGaA, Institute of Toxicology, Darmstadt, Germany
SO Naunyn-Schmiedeberg's Archives of Pharmacology, (March 2003) Vol. 367, No. Supplement 1, pp. R154. print.
Meeting Info.: 44th Spring Meeting of the Deutsche Gesellschaft fuer Experimentelle und Klinische Pharmakologie und Toxikologie and the 20th Meeting of the Gesellschaft fuer Umwelt-Mutationsforschung. Mainz, Germany. March 17-20, 2003.
ISSN: 0028-1298 (ISSN print).
DT Conference; (Meeting)
Conference; Abstract; (Meeting Abstract)
LA English
ED Entered STN: 2 Jul 2003
Last Updated on STN: 2 Jul 2003

L2 ANSWER 3 OF 18 MEDLINE on STN DUPLICATE 1
Full Text
AN 2002322867 MEDLINE
DN PubMed ID: 12065231
TI 6-Carboxymethyl genistein: a novel selective oestrogen receptor modulator (SERM) with unique, differential effects on the vasculature, bone and uterus.
AU Somjen D; Amir-Zaltsman Y; Gayer B; Kulik T; Knoll E; Stern N; Lu L J W; **Toldo L**; Kohen F
CS Department of BiologicalRegulation, Weizmann Institute of Science, Rehovot, 76100 Israel.
NC P30 ES 06676 (NIEHS)
SO Journal of endocrinology, (2002 Jun) 173 (3) 415-27.
Journal code: 0375363. ISSN: 0022-0795.
CY England: United Kingdom
DT Journal; Article; (JOURNAL ARTICLE)
LA English
FS Priority Journals

EM 200208
ED Entered STN: 20020615
Last Updated on STN: 20020810
Entered Medline: 20020809
AB The novel genistein (G) derivative, 6-carboxymethyl genistein (CG) was evaluated for its biological properties in comparison with G. Both compounds showed oestrogenic activity in vitro and in vivo. On the other hand G and CG differed in the following parameters: (i) only CG displayed mixed agonist-antagonist activity for oestrogen receptor (ER) alpha in transactivation assays and (ii) only CG was capable of attenuating oestrogen (E(2))-induced proliferation in vascular smooth muscle cells and of inhibiting oestrogen-induced creatine kinase (CK) specific activity in rat tissues. On the other hand only G enhanced the stimulatory effect on CK specific activity in the uterus. In comparison to the selective oestrogen receptor modulator (SERM) raloxifene (RAL), CG showed the same selectivity profile as RAL in blocking the CK response to E(2) in tissues derived from both immature and ovariectomized female rats. Molecular modelling of CG bound to the ligand binding domain (LBD) of ERbeta predicts that the 6-carboxymethyl group of CG almost fits the binding cavity. On the other hand, molecular modelling of CG bound to the LBD of ERalpha suggests that the carboxyl group of CG may perturb the end of Helix 11, eliciting a severe backbone change for Leu 525, and consequently induces a conformational change which could position Helix 12 in an antagonist conformation. This model supports the experimental findings that CG can act as a mixed agonist-antagonist when E(2) is bound to its receptors. Collectively, our findings suggest that CG can be considered a novel SERM with unique effects on the vasculature, bone and uterus.

L2 ANSWER 4 OF 18 MEDLINE on STN
Full Text
AN 2001102271 MEDLINE
DN PubMed ID: 10977085
TI An evaluation of ontology exchange languages for bioinformatics.
AU McEntire R; Karp P; Abernethy N; Benton D; Helt G; DeJongh M; Kent R; Kosky A; Lewis S; Hodnett D; Neumann E; Olken F; Pathak D; Tarczy-Hornoch P; **Toldo L**; Topaloglou T
CS SmithKline Beecham Pharmaceuticals, King of Prussia, PA 19406, USA.. Robin A McEntire@sbphrd.com
SO Proceedings / ... International Conference on Intelligent Systems for Molecular Biology ; ISMB. International Conference on Intelligent Systems for Molecular Biology, (2000) 8 239-50.
Journal code: 9509125.
CY United States
DT Journal; Article; (JOURNAL ARTICLE)
LA English
FS Priority Journals
EM 200101
ED Entered STN: 20010322
Last Updated on STN: 20010322
Entered Medline: 20010126
AB Ontologies are specifications of the concepts in a given field, and of the relationships among those concepts. The development of ontologies for molecular-biology information and the sharing of those ontologies within the bioinformatics community are central problems in bioinformatics. If the bioinformatics community is to share ontologies effectively, ontologies must be exchanged in a form that uses standardized syntax and semantics. This paper reports on an effort among the authors to evaluate alternative ontology-exchange languages, and to recommend one or more languages for use within the larger bioinformatics community. The study selected a set of candidate languages, and defined a set of capabilities

that the ideal ontology-exchange language should satisfy. The study scored the languages according to the degree to which they satisfied each capability. In addition, the authors performed several ontology-exchange experiments with the two languages that received the highest scores: OML and Ontolingua. The result of those experiments, and the main conclusion of this study, was that the frame-based semantic model of Ontolingua is preferable to the conceptual graph model of OML, but that the XML-based syntax of OML is preferable to the Lisp-based syntax of Ontolingua.

L2 ANSWER 5 OF 18 MEDLINE on STN
Full Text
AN 2000139296 MEDLINE
DN PubMed ID: 10681126
TI Web alert. Cell differentiation cell multiplication.
AU Pines J; **Toldo L**; Lafont F
CS Welcome/CRC Institute, Cambridge, UK.
SO Current opinion in cell biology, (1999 Dec) 11 (6) 651-2.
Journal code: 8913428. ISSN: 0955-0674.
CY United States
DT (DIRECTORY)
LA English
FS Priority Journals
EM 200002
ED Entered STN: 20000229
Last Updated on STN: 20000229
Entered Medline: 20000215

L2 ANSWER 6 OF 18 MEDLINE on STN
Full Text
AN 2000066494 MEDLINE
DN PubMed ID: 10610095
TI Cell-to-cell contact and extracellular matrix. Web Alert.
AU Pines J; **Toldo L**; Lafont F
CS Wellcome/CRC Institute, Campbridge, UK. JP103@mole.bio.cam.ac.uk
SO Current opinion in cell biology, (1999 Oct) 11 (5) 535-6.
Journal code: 8913428. ISSN: 0955-0674.
CY United States
DT (DIRECTORY)
LA English
FS Priority Journals
EM 199912
ED Entered STN: 20000113
Last Updated on STN: 20000124
Entered Medline: 19991216

L2 ANSWER 7 OF 18 MEDLINE on STN
Full Text
AN 1999347318 MEDLINE
DN PubMed ID: 10428544
TI Nucleus and gene expression. Web alert.
AU Pines J; **Toldo L**; Lafont F
CS Wellcome/CRC Institute, Cambridge, UK.. JP103@mole.bio.cam.ac.uk
SO Current opinion in cell biology, (1999 Jun) 11 (3) 301.
Journal code: 8913428. ISSN: 0955-0674.
CY United States
DT (DIRECTORY)
LA English
FS Priority Journals
EM 199907
ED Entered STN: 19990806

Last Updated on STN: 19990806
Entered Medline: 19990723

L2 ANSWER 8 OF 18 MEDLINE on STN
Full Text
AN 1999178217 MEDLINE
DN PubMed ID: 10084795
TI Cytoskeleton. Web alert.
AU Pines J; **Toldo L**; Lafont F
CS Wellcome/CRC Institute, Cambridge, UK.. JP103@mole.bio.cam.ac.uk
SO Current opinion in cell biology, (1999 Feb) 11 (1) 11-3.
Journal code: 8913428. ISSN: 0955-0674.
CY United States
DT (DIRECTORY)
LA English
FS Priority Journals
EM 199903
ED Entered STN: 19990326
Last Updated on STN: 20000124
Entered Medline: 19990316

L2 ANSWER 9 OF 18 MEDLINE on STN
Full Text
AN 1999136946 MEDLINE
DN PubMed ID: 9988534
TI Cell differentiation. Cell multiplication. Web alert.
AU Pines J; **Toldo L**; Lafont F
CS Wellcome/CRC Institute, Cambridge, UK.. JP103@mole.bio.cam.ac.uk
SO Current opinion in cell biology, (1998 Dec) 10 (6) 683-4.
Journal code: 8913428. ISSN: 0955-0674.
CY United States
DT (DIRECTORY)
LA English
FS Priority Journals
EM 199902
ED Entered STN: 19990223
Last Updated on STN: 20000303
Entered Medline: 19990209

L2 ANSWER 10 OF 18 MEDLINE on STN
Full Text
AN 1999085838 MEDLINE
DN PubMed ID: 9874581
TI Cell to cell contact and extracellular matrix.
AU Pines J; **Toldo L**; Lafont F
CS Wellcome/CRS Institute, Cambridge, UK.. jp103@mole.bio.cam.ac
SO Current opinion in cell biology, (1998 Oct) 10 (5) 561.
Journal code: 8913428. ISSN: 0955-0674.
CY United States
DT (DIRECTORY)
LA English
FS Priority Journals
EM 199812
ED Entered STN: 19990115
Last Updated on STN: 19990115
Entered Medline: 19981229

L2 ANSWER 11 OF 18 MEDLINE on STN
Full Text
AN 1998386329 MEDLINE

DN PubMed ID: 9719860
TI Membrane permeability. Membranes and sorting.
AU Pines J; **Toldo L**; Lafont F
CS Wellcome/CRC Institute, Cambridge.. JP103@mole.cam.ac.uk
SO Current opinion in cell biology, (1998 Aug) 10 (4) 427-8.
Journal code: 8913428. ISSN: 0955-0674.
CY United States
DT (DIRECTORY)
LA English
FS Priority Journals
EM 199812
ED Entered STN: 19990115
Last Updated on STN: 19990115
Entered Medline: 19981222

L2 ANSWER 12 OF 18 MEDLINE on STN
Full Text
AN 1998222651 MEDLINE
DN PubMed ID: 9561838
TI Cell regulation web alert.
AU **Toldo L**; Lafont F
CS MERCK KGaA, Bio- and Chemoinformatics, Darmstadt, Germany..
luca.toldo@merck.de
SO Current opinion in cell biology, (1998 Apr) 10 (2) 155.
Journal code: 8913428. ISSN: 0955-0674.
CY United States
DT (DIRECTORY)
LA English
FS Priority Journals
EM 199806
ED Entered STN: 19980625
Last Updated on STN: 20000303
Entered Medline: 19980618

L2 ANSWER 13 OF 18 MEDLINE on STN DUPLICATE 2
Full Text
AN 97429414 MEDLINE
DN PubMed ID: 9283764
TI JaMBW 1.1: Java-based Molecular Biologists' Workbench.
AU **Toldo L I**
CS MERCK KGaA, Darmstadt, Germany.. luca.toldo@merck.de
SO Computer applications in the biosciences : CABIOS, (1997 Aug) 13 (4)
475-6.
Journal code: 8511758. ISSN: 0266-7061.
CY ENGLAND: United Kingdom
DT Journal; Article; (JOURNAL ARTICLE)
LA English
FS Priority Journals
EM 199710
ED Entered STN: 19971105
Last Updated on STN: 19971105
Entered Medline: 19971023

L2 ANSWER 14 OF 18 MEDLINE on STN
Full Text
AN 97303153 MEDLINE
DN PubMed ID: 9159087
TI Web alert. Nucleus and gene expression.
AU Pines J; **Toldo L**; Lafont F
CS Wellcome/CRC Institute, Tennis Court Road, Cambridge, CB2 1QR, UK..

JP103@mole.bio.cam.ac.uk
SO Current opinion in cell biology, (1997 Jun) 9 (3) 431.
Journal code: 8913428. ISSN: 0955-0674.
CY United States
DT (DIRECTORY)
LA English
FS Priority Journals
EM 199708
ED Entered STN: 19970902
Last Updated on STN: 20000303
Entered Medline: 19970818

L2 ANSWER 15 OF 18 MEDLINE on STN
Full Text
AN 97224252 MEDLINE
DN PubMed ID: 9069269
TI Web alert. Cell regulation.
AU Pines J; **Toldo L**; Lafont F
CS Wellcome/CRC Institute, Tennis Court Road, Cambridge, CB2 1QR, UK..
JP103@mole.bio.cam.ac.uk
SO Current opinion in cell biology, (1997 Apr) 9 (2) 253-4.
Journal code: 8913428. ISSN: 0955-0674.
CY United States
DT (DIRECTORY)
LA English
FS Priority Journals
EM 199704
ED Entered STN: 19970506
Last Updated on STN: 20000303
Entered Medline: 19970423

L2 ANSWER 16 OF 18 MEDLINE on STN
Full Text
AN 97186505 MEDLINE
DN PubMed ID: 9035697
TI Web alert. Cytoskeleton.
AU Lafont F; **Toldo L**
CS Cell Biology Programme, European Molecular Biology Laboratory,
Meyerhofstrasse 1, Heidelberg 69012, Germany.. lafont@EMBL-heidelberg.de
SO Current opinion in cell biology, (1997 Feb) 9 (1) 118.
Journal code: 8913428. ISSN: 0955-0674.
CY United States
DT (DIRECTORY)
LA English
FS Priority Journals
EM 199702
ED Entered STN: 19970306
Last Updated on STN: 20000303
Entered Medline: 19970227

L2 ANSWER 17 OF 18 MEDLINE on STN
Full Text
AN 97186504 MEDLINE
DN PubMed ID: 9035696
TI The cell biologist and the World Wide Web. World Wide Web sites.
AU Lafont F; **Toldo L**
CS Cell Biology Programme, European Molecular Biology Laboratory,
Meyerhofstrasse 1, Heidelberg 69012, Germany.. lafont@EMBL-heidelberg.de
SO Current opinion in cell biology, (1997 Feb) 9 (1) 116-7. Ref: 2
Journal code: 8913428. ISSN: 0955-0674.

CY United States
DT Journal; Article; (JOURNAL ARTICLE)
General Review; (REVIEW)
(REVIEW, TUTORIAL)
LA English
FS Priority Journals
EM 199702
ED Entered STN: 19970306
Last Updated on STN: 19970306
Entered Medline: 19970227

L2 ANSWER 18 OF 18 MEDLINE on STN DUPLICATE 3
Full Text
AN 89275506 MEDLINE
DN PubMed ID: 2659222
TI Somatotropin as measured by a two-site time-resolved immunofluorometric assay.
CM Comment in: Clin Chem. 1990 Feb;36(2):402. PubMed ID: 2302801
AU Strasburger C; Barnard G; **Toldo L**; Zarmi B; Zadik Z; Kowarski A; Kohen F
CS Department of Hormone Research, Weizmann Institute of Science, Rehovot, Israel.
SO Clinical chemistry, (1989 Jun) 35 (6) 913-7.
Journal code: 9421549. ISSN: 0009-9147.
CY United States
DT Journal; Article; (JOURNAL ARTICLE)
LA English
FS Priority Journals
EM 198907
ED Entered STN: 19900309
Last Updated on STN: 19900309
Entered Medline: 19890721
AB To date, many of the current criteria for diagnosis of somatotropin (growth hormone, GH) deficiency have been based upon measurement of this hormone by competitive radioimmunoassay (RIA) with use of polyclonal antibodies. In recent years, however, the development of hybridoma technology has led to the generation of various monoclonal antibodies (Mabs) to GH with different affinities and epitope specificities. Subsequently, these reagents have been used in the development of noncompetitive two-site immunometric assays (e.g., immunoradiometric assay; IRMA). In general, the values obtained for serum GH by IRMA have been lower than those obtained by RIA, because of the epitope-specificity profile of the Mabs in the IRMA. Attempting to obtain GH values numerically similar to those by RIA, we used a combination of Mabs to GH in developing and evaluating a two-site time-resolved immunofluorometric assay (IFMA) based on the streptavidin-biotin interaction. Fluorescence is proportional to concentration of analyte and is linearly related to concentration over the range 0.3 to 40 micrograms/L. The assay was satisfactory with respect to sensitivity, accuracy, and precision (CV less than 10% over the entire working range). In addition, the concentration of GH was determined by the IFMA and a competitive RIA in serum obtained from GH deficient and acromegalic patients. The pairing of antibodies in the IFMA gave numerical values that agreed well with those by RIA (r = 0.97; n = 100).

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E14 46 RIPPMANN E T/AU
E15 22 --> RIPPMANN F/AU
E16 10 RIPPMANN FRIEDRICH/AU

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E21          1     RIPPMANN P/AU
E22          2     RIPPMANN V/AU
E23          1     RIPPMANN VOLKER/AU
E24          1     RIPPO A/AU

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L3          32 ("RIPPMANN F"/AU OR "RIPPMANN FRIEDRICH"/AU)

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DUPLICATE PREFERENCE IS 'MEDLINE, BIOSIS'
KEEP DUPLICATES FROM MORE THAN ONE FILE?  Y/(N):n
PROCESSING COMPLETED FOR L3
L4           25 DUPLICATE REMOVE L3 (7 DUPLICATES REMOVED)

=> d 1-25 bib ab

L4   ANSWER 1 OF 25  BIOSIS  COPYRIGHT 2004 BIOLOGICAL ABSTRACTS INC. on STN
Full Text
AN   2003:266107  BIOSIS
DN   PREV200300266107
TI   Bicyclic amino acids.
AU   Diefenbach, Beate [Inventor, Reprint Author]; Goodman, Simon L.
     [Inventor]; Marz, Joachim [Inventor]; Raddatz, Peter [Inventor];
     Rippmann, Friedrich [Inventor]; Wiesner, Matthias [Inventor]
CS   Darmstadt, Germany
     ASSIGNEE: Merck Patent Gesellschaft Mit, Darmstadt, Germany
PI   US 6559144 May 06, 2003
SO   Official Gazette of the United States Patent and Trademark Office Patents,
     (May 6 2003) Vol. 1270, No. 1. http://www.uspto.gov/web/menu/patdata.html.
     e-file.
     ISSN: 0098-1133 (ISSN print).
DT   Patent
LA   English
ED   Entered STN: 4 Jun 2003
     Last Updated on STN: 4 Jun 2003
AB   Compounds of the formula I ##STR1## in which X, Y, Z, R1, R2, R3, R4, R5,
     R7, R8, R11, m and n have the meanings stated in claim 1, and their
     physiologically acceptable salts can be used as integrin inhibitors, in
     particular for the prophylaxis and treatment of circulatory disorders, for
     thrombosis, myocardial infarct, coronary heart disease, arteriosclerosis,
     osteoporosis, for pathological processes maintained or propagated by
     angiogenesis, and in tumour therapy.

L4   ANSWER 2 OF 25     MEDLINE on STN                    DUPLICATE 1
Full Text
AN   2002454952     MEDLINE
DN   PubMed ID: 12213573
TI   Divalent cations and the relationship between alphaA and betaA domains in
     integrins.
AU   Seow Kah-Tong; Xiong Jian-Ping; Arnaout M Amin; Welge Jutta; Rippmann
     Friedrich; Goodman Simon L
CS   Department of Bio- and Chemoinformatics, Merck KGaA, Frankfurterstr. 250,
     Darmstadt, Germany.
SO   Biochemical pharmacology, (2002 Sep) 64 (5-6) 805-12.
     Journal code: 0101032. ISSN: 0006-2952.
CY   England: United Kingdom
```

DT Journal; Article; (JOURNAL ARTICLE)
LA English
FS Priority Journals
EM 200210
ED Entered STN: 20020906
Last Updated on STN: 20021018
Entered Medline: 20021017
AB Integrins contain either one or two von Willebrand factor A-like domains, which are primary ligand and cation binding regions in the molecules. Here we examine the first structure of an A domain of a beta subunit, in alphanubeta3 and compare it to known A domain structures of alpha subunits. Ligand binding to immobilized alphanubeta3 domain is stimulated by Ca2+ rather than inhibited by it. Biochemical, cell biological and structural evidence suggests that the A domain is a major site of ligand interaction in alphanubeta3. The Arg-Gly-Asp based inhibitor cilengitide (EMD 121974) inhibites ligand interaction with transmembrane-truncated alphanubeta3 in the presence of either Ca2+ or Mn2+ ions, and does so with similar kinetics. The alphanubeta3 structure reveals that both the alphaA and betaA domains share common structural cores. But, in contrast to alphaA, the betaA domain has three cation binding sites, that are involved either directly or indirectly in ligand binding. Structural alignment of alphaA and betaA domains reveals additional loops unique only to the betaA domain and much evidence support that that these loops are important for ligand binding specificity and for the interaction between alpha and beta subunits. Since the position of these loops are evolutionary conserved but their primary sequence varies between the various betaA domains, they represents potential targets for dissecting functional diversity among integrins.

L4 ANSWER 3 OF 25 BIOSIS COPYRIGHT 2004 BIOLOGICAL ABSTRACTS INC. on STN
Full Text
AN 2001:296926 BIOSIS
DN PREV200100296926
TI Cyclic adhesion inhibitors.
AU Jonczyk, Alfred [Inventor, Reprint author]; Holzemann, Gunter [Inventor]; Felding-Habermann, Brunhilde [Inventor]; **Rippmann, Friedrich** [Inventor]; Diefenbach, Beate [Inventor]; Kessler, Horst [Inventor]; Haubner, Roland [Inventor]; Wermuth, Jochen [Inventor]
CS Darmstadt, Germany
ASSIGNEE: Merck Patent Gesellschaft Mit, Germany
PI US 6169072 January 02, 2001
SO Official Gazette of the United States Patent and Trademark Office Patents, (Jan. 2, 2001) Vol. 1242, No. 1. e-file.
CODEN: OGUPE7. ISSN: 0098-1133.
DT Patent
LA English
ED Entered STN: 20 Jun 2001
Last Updated on STN: 19 Feb 2002
AB The invention relates to novel cyclopeptides of the formula I cyclo-(Arg-B-Asp-D-E) I in which B, D, and E have the meanings defined herein, and their salts. These compounds act as interin inhibitors and can be used, in particular, for the prophylaxis and treatment of disorders of the circulation and in tumor therapy.

L4 ANSWER 4 OF 25 BIOSIS COPYRIGHT 2004 BIOLOGICAL ABSTRACTS INC. on STN
Full Text
AN 1999:71973 BIOSIS
DN PREV199900071973
TI Cyclic peptides containing Arg-Gly-Asp, and derivatives thereof, as adhesion inhibitors.

AU Jonczyk, A. [Inventor]; Holzemann, G. [Inventor]; Felding-Habermann, B. [Inventor]; **Rippmann, F.** [Inventor]; Diefenbach, B. [Inventor]; Kessler, H. [Inventor]; Haubner, R. [Inventor]; Wermuth, J. [Inventor]
CS Darmstadt, Germany
ASSIGNEE: MERCK PATENT GESELLSCHAFT MIT BESCHRANKTER HAFTUNG
PI US 5849692 Dec. 15, 1998
SO Official Gazette of the United States Patent and Trademark Office Patents, (Dec. 15, 1998) Vol. 1217, No. 3, pp. 2573. print.
CODEN: OGUPE7. ISSN: 0098-1133.
DT Patent
LA English
ED Entered STN: 1 Mar 1999
Last Updated on STN: 1 Mar 1999

L4 ANSWER 5 OF 25 BIOSIS COPYRIGHT 2004 BIOLOGICAL ABSTRACTS INC. on STN
Full Text
AN 2002:107001 BIOSIS
DN PREV200200107001
TI Linear adhesion inhibitors.
AU Jonczyk, A. [Inventor]; Felding-Habermann, B. [Inventor]; Diefenbachh, B. [Inventor]; **Rippmann, F.** [Inventor]
CS Darmstadt, Germany
ASSIGNEE: MERCK PATENT GESELLSCHAFT MIT BESCHRANKTER HAFTUNG
PI US 5747457 May 5, 1998
SO Official Gazette of the United States Patent and Trademark Office Patents, (May 5, 1998) Vol. 1210, No. 1, pp. 493-494. print.
CODEN: OGUPE7. ISSN: 0098-1133.
DT Patent
LA English
ED Entered STN: 24 Jan 2002
Last Updated on STN: 26 Feb 2002

L4 ANSWER 6 OF 25 BIOSIS COPYRIGHT 2004 BIOLOGICAL ABSTRACTS INC. on STN
Full Text
AN 2002:89701 BIOSIS
DN PREV200200089701
TI Cyclopeptides.
AU Jonczyk, A. [Inventor]; Holzermann, G. [Inventor]; Felding-Habermann, B. [Inventor]; **Rippmann, F.** [Inventor]; Melzer, G. [Inventor]; Diefenbach, B. [Inventor]
CS Darmstadt, Germany
ASSIGNEE: MERCK PATENT GESELLSCHAFT MIT BESCHRANKTER HAFTUNG
PI US 5705481 Jan. 6, 1998
SO Official Gazette of the United States Patent and Trademark Office Patents, (Jan. 6, 1998) Vol. 1206, No. 1, pp. 472-11. print.
CODEN: OGUPE7. ISSN: 0098-1133.
DT Patent
LA English
ED Entered STN: 16 Jan 2002
Last Updated on STN: 25 Feb 2002

L4 ANSWER 7 OF 25 MEDLINE on STN
Full Text
AN 1998369921 MEDLINE
DN PubMed ID: 9704298
TI LIGSITE: automatic and efficient detection of potential small molecule-binding sites in proteins.
AU Hendlich M; **Rippmann F**; Barnickel G
CS Department of Pharmaceutical Chemistry, University of Marburg, Germany.
SO Journal of molecular graphics & modelling, (1997 Dec) 15 (6) 359-63, 389.

Journal code: 9716237. ISSN: 1093-3263.
CY United States
DT Journal; Article; (JOURNAL ARTICLE)
LA English
FS Priority Journals
EM 199810
ED Entered STN: 19990106
Last Updated on STN: 19990106
Entered Medline: 19981023
AB LIGSITE is a new program for the automatic and time-efficient detection of pockets on the surface of proteins that may act as binding sites for small molecule ligands. Pockets are identified with a series of simple operations on a cubic grid. Using a set of receptor-ligand complexes we show that LIGSITE is able to identify the binding sites of small molecule ligands with high precision. The main advantage of LIGSITE is its speed. Typical search times are in the range of 5 to 20 s for medium-sized proteins. LIGSITE is therefore well suited for identification of pockets in large sets of proteins (e.g., protein families) for comparative studies. For graphical display LIGSITE produces VRML representations of the protein-ligand complex and the binding site for display with a VRML viewer such as WebSpace from SGI.

L4 ANSWER 8 OF 25 BIOSIS COPYRIGHT 2004 BIOLOGICAL ABSTRACTS INC. on STN
Full Text
AN 1996:487627 BIOSIS
DN PREV199699209983
TI Sequence-function correlation in G protein-coupled receptors.
AU Kuipers, W. [Reprint author]; Oliveira, L.; Paiva, A. C. M.; **Rippmann, F.**; Sander, C.; Vriend, G.; Ijzerman, A. P.
CS Dep. Med. Chem., Solvay Duphar B.V., P.O. Box 900, NL-1380 DA Weesp, Netherlands
SO Findlay, J. B. C. [Editor]. (1996) pp. 27-45. Membrane proteins models. Publisher: BIOS Scientific Publishers Ltd., St. Thomas House, Becket Street, Oxford OX1 ISJ, England.
Meeting Info.: Conference on Membrane Protein Models: Experiment, Theory, and Speculation. Leeds, England, UK. March 1994; April 1994.
ISBN: 1-85996-080-4.
DT Book
Conference; (Meeting)
Book; (Book Chapter)
Conference; (Meeting Paper)
LA English
ED Entered STN: 4 Nov 1996
Last Updated on STN: 5 Nov 1996

L4 ANSWER 9 OF 25 BIOSIS COPYRIGHT 2004 BIOLOGICAL ABSTRACTS INC. on STN
Full Text
AN 1996:487631 BIOSIS
DN PREV199699209987
TI Pride and prejudice and G protein-coupled receptor models.
AU **Rippmann, Friedrich**
CS E. Merck, Preclin. Pharm. Res., D-64271 Darmstadt, Germany
SO Findlay, J. B. C. [Editor]. (1996) pp. 91-112. Membrane proteins models. Publisher: BIOS Scientific Publishers Ltd., St. Thomas House, Becket Street, Oxford OX1 ISJ, England.
Meeting Info.: Conference on Membrane Protein Models: Experiment, Theory, and Speculation. Leeds, England, UK. March 1994; April 1994.
ISBN: 1-85996-080-4.
DT Book
Conference; (Meeting)

Book; (Book Chapter)
Conference; (Meeting Paper)
LA English
ED Entered STN: 4 Nov 1996
Last Updated on STN: 4 Nov 1996

L4 ANSWER 10 OF 25 BIOSIS COPYRIGHT 2004 BIOLOGICAL ABSTRACTS INC. on STN
Full Text
AN 1996:541758 BIOSIS
DN PREV199699264114
TI New antithrombotic RGD-mimetics with high bioavailability.
AU Gante, Joachim [Reprint author]; Juraszyk, Horst; Raddatz, Peter; Wurziger, Hanns; Bernotat-Danielowski, Sabine; Melzer, Guido; **Rippmann, Friedrich**
CS Merck KGaA, Preclinical Res. Dep., Frankfurter Str. 250, D-64271 Darmstadt, Germany
SO Bioorganic and Medicinal Chemistry Letters, (1996) Vol. 6, No. 20, pp. 2425-2430.
CODEN: BMCLE8. ISSN: 0960-894X.
DT Article
LA English
ED Entered STN: 10 Dec 1996
Last Updated on STN: 10 Dec 1996
AB A new class of antithrombotic RGD-mimetics with a novel oxazolidinonemethyl scaffold was synthesized. High oral activity and bioavailability was found in this series of compounds.

L4 ANSWER 11 OF 25 MEDLINE on STN DUPLICATE 2
Full Text
AN 96013822 MEDLINE
DN PubMed ID: 7474139
TI An active-site mutation in the human immunodeficiency virus type 1 proteinase (PR) causes reduced PR activity and loss of PR-mediated cytotoxicity without apparent effect on virus maturation and infectivity.
AU Konvalinka J; Litterst M A; Welker R; Kottler H; **Rippmann F**; Heuser A M; Krausslich H G
CS Angewandte Tumorvirologie, Deutsches Krebsforschungszentrum, Heidelberg, Germany.
SO Journal of virology, (1995 Nov) 69 (11) 7180-6.
Journal code: 0113724. ISSN: 0022-538X.
CY United States
DT Journal; Article; (JOURNAL ARTICLE)
LA English
FS Priority Journals; AIDS
EM 199512
ED Entered STN: 19960124
Last Updated on STN: 19970203
Entered Medline: 19951201
AB Infectious retrovirus particles are derived from structural polyproteins which are cleaved by the viral proteinase (PR) during virion morphogenesis. Besides cleaving viral polyproteins, which is essential for infectivity, PR of human immunodeficiency virus (HIV) also cleaves cellular proteins and PR expression causes a pronounced cytotoxic effect. Retroviral PRs are aspartic proteases and contain two copies of the triplet Asp-Thr-Gly in the active center with the threonine adjacent to the catalytic aspartic acid presumed to have an important structural role. We have changed this threonine in HIV type 1 PR to a serine. The purified mutant enzyme had an approximately 5- to 10-fold lower activity against HIV type 1 polyprotein and peptide substrates compared with the wild-type enzyme. It did not induce toxicity on bacterial expression and yielded

significantly reduced cleavage of cytoskeletal proteins in vitro. Cleavage of vimentin in mutant-infected T-cell lines was also markedly reduced. Mutant virus did, however, elicit productive infection of several T-cell lines and of primary human lymphocytes with no significant difference in polyprotein cleavage and with similar infection kinetics and titer compared with wild-type virus. The discrepancy between reduced processing in vitro and normal virion maturation can be explained by the observation that reduced activity was due to an increase in Km which may not be relevant at the high substrate concentration in the virus particle. This mutation enables us therefore to dissociate the essential function of PR in viral maturation from its cytotoxic effect.

L4 ANSWER 12 OF 25 BIOSIS COPYRIGHT 2004 BIOLOGICAL ABSTRACTS INC. on STN
Full Text
AN 1996:479751 BIOSIS
DN PREV199699195007
TI New peptidomimetics in the chemistry of fibrinogen receptor antagonists.
AU Gante, J. [Reprint author]; Juraszyk, H.; Raddatz, P.; Wurziger, H.; Bernotat-Danielowski, S.; Melzer, G.; **Rippmann, F.**
CS Merck KGaA, Preclinical Pharmaceutical Res. Dep., Frankfurter Strasse 250, D-64271 Darmstadt, Germany
SO Letters in Peptide Science, (1995) Vol. 2, No. 3-4, pp. 135-140. ISSN: 0929-5666.
DT Article
LA English
ED Entered STN: 24 Oct 1996
Last Updated on STN: 24 Oct 1996
AB RGD-peptidomimetics are currently being investigated as a class of potential antithrombotics that antagonize the fibrinogen receptor, GP IIb/IIIa, on the surface of platelets. These mimetics are expected to have decisive advantages - such as higher activity and specificity, oral bioavailability and longer duration of action - over known antithrombotics. For further optimization in this respect, novel peptidomimetic GP IIb/IIIa antagonists with an oxazolidinonemethyl central building block were synthesized. This building block proved to be very versatile as an 'anchor' for structurally different C-termini and was the starting point for highly efficient and orally active compounds.

L4 ANSWER 13 OF 25 MEDLINE on STN DUPLICATE 3
Full Text
AN 94166050 MEDLINE
DN PubMed ID: 8120867
TI Non-peptide renin inhibitors containing 2-(((3-phenylpropyl)phosphoryl)oxy)alkanoic acid moieties as P2-P3 replacements.
AU Raddatz P; Minck K O; **Rippmann F**; Schmitges C J
CS E. Merck Darmstadt, Germany.
SO Journal of medicinal chemistry, (1994 Feb 18) 37 (4) 486-97. Journal code: 9716531. ISSN: 0022-2623.
CY United States
DT Journal; Article; (JOURNAL ARTICLE)
LA English
FS Priority Journals
EM 199404
ED Entered STN: 19940412
Last Updated on STN: 19940412
Entered Medline: 19940407
AB A series of novel renin inhibitors containing 2-(((3-phenylpropyl)phosphoryl)oxy)alkanoic acid moieties as P2-P3 surrogates are presented. The P2-P3 mimetics were obtained from (omega-phenylalkyl)-phosphinic acids 1a-c and 2-hydroxyalkanoic acid benzyl esters 2a-f by

N,N'-dicyclohexylcarbodiimide-mediated coupling and subsequent oxidation with sodium metaperjodate. Ester cleavage of these derivatives and coupling with P1-P1' transition-state mimetics I-VII provided highly selective compounds with inhibitory potencies in the lower nanomolar range. Small renin inhibitors, such as analogues 8c and 8h with molecular weights of 539 and 537, respectively, could be prepared. These compounds exhibited IC50 values of about 20 nM against human plasma renin. Compound 7i was examined in vivo for its hypotensive effect. In salt-depleted cynomolgus monkeys, 7i inhibited plasma renin activity almost completely and lowered blood pressure after oral administration of a dose of 30 mg/kg.

L4 ANSWER 14 OF 25 BIOSIS COPYRIGHT 2004 BIOLOGICAL ABSTRACTS INC. on STN
Full Text
AN 1994:326901 BIOSIS
DN PREV199497339901
TI Analysis of temperature-sensitive mutants of HIV-1 proteinase.
AU Konvalinka, Jan [Reprint author]; Kottler, Hubert; **Rippmann, Friedrich**; Kraeusslich, Hans-Georg
CS Angewandte Tumorvirologie, Deutsches Krebsforschungszentrum, D-69120 Heidelberg, Germany
SO Journal of Cellular Biochemistry Supplement, (1994) Vol. 0, No. 18D, pp. 169.
Meeting Info.: Keystone Symposium on Structural and Molecular Biology of Protease Function and Inhibition. Santa Fe, New Mexico, USA. March 5-12, 1994.
ISSN: 0733-1959.
DT Conference; (Meeting)
Conference; Abstract; (Meeting Abstract)
Conference; (Meeting Poster)
LA English
ED Entered STN: 2 Aug 1994
Last Updated on STN: 3 Aug 1994

L4 ANSWER 15 OF 25 BIOSIS COPYRIGHT 2004 BIOLOGICAL ABSTRACTS INC. on STN
Full Text
AN 1994:144259 BIOSIS
DN PREV199497157259
TI Peptides from the second calcium binding domain of integrin chain alpha-IIb inhibit fibrinogen binding to alpha-IIb-beta-3 by direct interaction.
AU Diefenbach, Beate [Reprint author]; Felding-Habermann, Brunhilde; Jonczyk, Alfred; **Rippmann, Friedrich** [Reprint author]
CS Preclin. Res., E. Merck, 64271 Darmstadt, Germany
SO Preissner, K. T. [Editor]; Rosenblatt, S. [Editor]; Kost, C. [Editor]; Wegerhoff, J. [Editor]; Mosher, D. F. [Editor]. Int. Congr. Ser. - Excerpta Med., (1993) pp. 149-156. International Congress Series; Biology of vitronectins and their receptors.
Publisher: Elsevier Science Publishers B.V., PO Box 211, Sara Burgerhartstraat 25, 1000 AE Amsterdam, Netherlands; Elsevier Science Publishing Co., Inc., P.O. Box 882, Madison Square Station, New York, New York 10159-2101, USA. Series: International Congress Series.
Meeting Info.: First International Vitronectin Workshop. Marburg, Germany. August 25-28, 1993.
CODEN: EXMDA4. ISSN: 0531-5131. ISBN: 0-444-81680-1.
DT Book
Conference; (Meeting)
Book; (Book Chapter)
Conference; (Meeting Paper)
LA English

ED Entered STN: 30 Mar 1994
Last Updated on STN: 31 Mar 1994

L4 ANSWER 16 OF 25 MEDLINE on STN DUPLICATE 4
Full Text
AN 93020916 MEDLINE
DN PubMed ID: 1404233
TI Renin inhibitors containing new P1-P1' dipeptide mimetics with heterocycles in P1'.
AU Raddatz P; Jonczyk A; Minck K O; **Rippmann F**; Schittenhelm C; Schmitges C J
CS E. Merck Darmstadt, Preclinical Pharmaceutical Research, Germany.
SO Journal of medicinal chemistry, (1992 Sep 18) 35 (19) 3525-36.
Journal code: 9716531. ISSN: 0022-2623.
CY United States
DT Journal; Article; (JOURNAL ARTICLE)
LA English
FS Priority Journals
EM 199210
ED Entered STN: 19930122
Last Updated on STN: 19930122
Entered Medline: 19921026
AB A series of renin inhibitors containing new P1-P1' dipeptide mimetics are presented. The P1-P1' mimetics were obtained from (4S,5S)-3-(tert-butoxycarbonyl)-4-(cyclohexylmethyl)-5-[(omega- mesyloxy)alkyl]-2,2-dimethyloxazolidines 5b, 9, and 11b by nucleophilic substitution of the mesylate groups with the sodium salts of mercapto- and hydroxyheterocycles. Removal of the protecting groups and stepwise acylations with amino acid derivatives provided renin inhibitors with a length of a tripeptide. Replacement of P2 histidine by other amino acids maintained or enhanced renin inhibitory potency. By alteration of P3 phenylalanine, compounds with IC50 values in the nanomolar range and stability against chymotrypsin were obtained. Finally, the effect of the C-terminal heterocycle on the renin inhibition was studied. Compound XVII was examined in vivo for its hypotensive effects. In salt-depleted cynomolgus monkeys, XVII inhibited plasma renin activity and lowered blood pressure after oral administration of a dose of 10 mg/kg.

L4 ANSWER 17 OF 25 MEDLINE on STN DUPLICATE 5
Full Text
AN 91216098 MEDLINE
DN PubMed ID: 2022182
TI A hypothetical model for the peptide binding domain of hsp70 based on the peptide binding domain of HLA.
AU **Rippmann F**; Taylor W R; Rothbard J B; Green N M
CS National Institute for Medical Research, Mill Hill, London, UK.
SO EMBO journal, (1991 May) 10 (5) 1053-9.
Journal code: 8208664. ISSN: 0261-4189.
CY ENGLAND: United Kingdom
DT Journal; Article; (JOURNAL ARTICLE)
LA English
FS Priority Journals
EM 199106
ED Entered STN: 19910623
Last Updated on STN: 19910623
Entered Medline: 19910605
AB The sequences of the peptide binding domains of 33 70 kd heat shock proteins (hsp70) have been aligned and a consensus secondary structure has been deduced. Individual members showed no significant deviation from the consensus, which showed a beta 4 alpha motif repeated twice, followed by two further helices and a terminus rich in Pro and Gly. The repeated

motif could be aligned with the secondary structure of the functionally equivalent peptide binding domain of human leucocyte antigen (HLA) class I maintaining equivalent residues in structurally important positions in the two families and a model was built based on this alignment. The interaction of this domain with the ATP domain is considered. The overall model is shown to be consistent with the properties of products of chymotryptic cleavage.

L4 ANSWER 18 OF 25 MEDLINE on STN
Full Text
AN 92254729 MEDLINE
DN PubMed ID: 1812738
TI Expression and characterization of genetically linked homo- and hetero-dimers of HIV proteinase.
AU Krausslich H G; Traenckner A M; **Rippmann F**
CS Institut fur Virusforschung/ATV, Deutsches Krebsforschungszentrum, Heidelberg.
SO Advances in experimental medicine and biology, (1991) 306 417-28. Journal code: 0121103. ISSN: 0065-2598.
CY United States
DT Journal; Article; (JOURNAL ARTICLE)
LA English
FS Priority Journals; AIDS
EM 199206
ED Entered STN: 19920619
Last Updated on STN: 19920619
Entered Medline: 19920610

L4 ANSWER 19 OF 25 MEDLINE on STN DUPLICATE 6
Full Text
AN 91236792 MEDLINE
DN PubMed ID: 2033089
TI Biological assays for irritant, tumor-initiating and -promoting activities. III. Computer-assisted management and validation of biodata generated by standardized initiation/promotion protocols in skin of mice.
AU Edler L; Schmidt R; Weber E; **Rippmann F**; Hecker E
CS Institute of Epidemiology and Biometry, German Cancer Research Center, Heidelberg.
SO Journal of cancer research and clinical oncology, (1991) 117 (3) 205-16. Journal code: 7902060. ISSN: 0171-5216.
CY GERMANY: Germany, Federal Republic of
DT Journal; Article; (JOURNAL ARTICLE)
LA English
FS Priority Journals
EM 199106
ED Entered STN: 19910714
Last Updated on STN: 19910714
Entered Medline: 19910621
AB The initiation/promotion standard protocol 28 (protocol 28), developed and used previously as an experimental model to verify the cancerogenic process of initiation/promotion in mouse skin, was revised in three aspects: (a) statistically it was shown sufficient to use, per promoter dose group, 16 colony-outbred female NMRI mice: (b) by weekly individual records of tumor response (and health status) of each mouse in a dose group, cumulative tumor incidences (and mean and extreme body weights) are determined; from these data the collective records (tumor response, health status), the only data accessible from protocol 28, may be generated in addition; (c) the details of dose groups and all data on tumor response and health status are processed by computer using the program package PAPILLOM. The latter was developed specifically for this purpose, is

written in the programming language APL and designed for easy handling by staff of animal laboratories. The program package calculates, from the individual records per promoter dose group, cumulative tumor incidences (and survival data) with confidence limits for any one exposure time, and the package may be linked to programs for statistical validations. In addition, from the collective records it calculates the tumor rates, tumor yields and survival rates for any one exposure time. These data, obtained by either of the standard protocols (16 or 28), are fully comparable. For pure compounds they may be used to calculate semiquantitative tumor-promoting potencies. These values for more than 80 polyfunctional diterpenes of the tigliane, ingenane and daphnane type, scattered in or calculated from previous papers, together with their irritancies, were compiled. Within recent years, computer-assisted standard protocol 16 has been used to handle and evaluate about 1000 promoter dose groups. Protocol 16 allows one to extract and utilize more and better toxicological information on tumor response and health status from any one dose group, utilizing significantly fewer experimental animals than required by protocol 28. Thus, the computer-assisted standard protocol 16 optimizes the utility of the experimental model of mouse skin for the amount, quality and management of experimental data as well as for the requirements of animal protection.

L4 ANSWER 20 OF 25 MEDLINE on STN
Full Text
AN 92126614 MEDLINE
DN PubMed ID: 1772839
TI Visualization of structural similarity in proteins.
AU **Rippmann F**; Taylor W R
CS Laboratory of Mathematical Biology, National Institute for Medical Research, London, UK.
SO Journal of molecular graphics, (1991 Sep) 9 (3) 169-74, 163-4.
Journal code: 9014762. ISSN: 0263-7855.
CY United States
DT Journal; Article; (JOURNAL ARTICLE)
LA English
FS Priority Journals
EM 199203
ED Entered STN: 19920322
Last Updated on STN: 19920322
Entered Medline: 19920304
AB Two new methods for the visualization of structural similarity in proteins with known three-dimensional structures are presented. They are based on the degree of equivalence of alpha-carbon pairs in two proteins. The quantitative measure for residue equivalence is the comparison score generated using the sequence and structure alignment method of Taylor and Orengo, which is based on the comparison of interatomic distances (and other properties that can be defined on a residue basis). The first method uses information on corresponding alpha-carbon positions to display vectors joining these structurally equivalent residues. These vectors can be defined as target constraints, and their minimization "bends" the two proteins toward a common average structure. In the average structure the corresponding residues virtually superpose, while insertions and deletions become clearly visible. The second method uses the comparison scores to perform a weighted least-squares fit of the two structures. It is further used to color code the two structures according to the score value, i.e., their similarity, on a continuous scale from red to blue. Examples of the methods for the comparison of flavodoxin, chemotaxis Y protein and L-arabinose-binding protein are given.

L4 ANSWER 21 OF 25 MEDLINE on STN DUPLICATE 7

Full Text
AN 92216408 MEDLINE
DN PubMed ID: 1806098
TI The application of a multistage model that incorporates DNA damage and repair to the analysis of initiation/promotion experiments.
AU Kopp-Schneider A; Portier C J; **Rippmann F**
CS Abteilung Biostatistik, Institut fur Epidemiologie und Biometrie, Deutsches Krebsforschungszentrum, Heidelberg, Germany.
SO Mathematical biosciences, (1991 Jul) 105 (2) 139-66.
Journal code: 0103146. ISSN: 0025-5564.
CY United States
DT Journal; Article; (JOURNAL ARTICLE)
LA English
FS Priority Journals
EM 199205
ED Entered STN: 19920529
Last Updated on STN: 19920529
Entered Medline: 19920514
AB In a previous article, a multistage model of carcinogenesis was introduced that takes into account the role of DNA damage, DNA repair, and cell replication on the incidence of malignancies. For this model the number of detectable clones of initiated cells is derived and model parameters are estimated using data arising from a two-stage skin-painting experiment in mice. The data from this experiment are interpretable in terms of the cellular events involved in initiation and promotion.

L4 ANSWER 22 OF 25 BIOSIS COPYRIGHT 2004 BIOLOGICAL ABSTRACTS INC. on STN
Full Text
AN 1991:194362 BIOSIS
DN PREV199140091642; BR40:91642
TI THRESHOLD DOSES FOR TELEOCIDIN AND OTHER ENVIRONMENTAL PROMOTERS OF MOUSE SKIN.
AU HECKER E [Reprint author]; **RIPPMANN F**; FUJIKI H
CS GERMAN CANCER RES CENTER, INST BIOCHEM, IM NEUENHEIMER FELD 280, D-6900 HEIDELBERG, FRG
SO Journal of Cancer Research and Clinical Oncology, (1990) Vol. 116, No. SUPPL. PART 2, pp. 1074.
Meeting Info.: 15TH INTERNATIONAL CANCER CONGRESS, HAMBURG, GERMANY, AUGUST 16-22, 1990. J CANCER RES CLIN ONCOL.
CODEN: JCROD7. ISSN: 0171-5216.
DT Conference; (Meeting)
FS BR
LA ENGLISH
ED Entered STN: 22 Apr 1991
Last Updated on STN: 14 Jun 1991

L4 ANSWER 23 OF 25 BIOSIS COPYRIGHT 2004 BIOLOGICAL ABSTRACTS INC. on STN
Full Text
AN 1990:333593 BIOSIS
DN PREV199090041612; BA90:41612
TI HYDROPHOBICITY AND TUMOR PROMOTING ACTIVITY OF PHORBOL ESTERS.
AU **RIPPMANN F** [Reprint author]
CS INST BIOCHEM, GER CANCER RES CENT, IM NEUENHEIMER FELD 280, D-6900 HEIDELBERG, W GER
SO Quantitative Structure-Activity Relationships, (1990) Vol. 9, No. 1, pp. 1-5.
CODEN: QSARDI. ISSN: 0931-8771.
DT Article
FS BA
LA ENGLISH

ED Entered STN: 24 Jul 1990
Last Updated on STN: 24 Jul 1990

AB Phorbol esters are polyfunctional agents which influence the carcinogenic process via a receptor mechanism. Two structural elements of phorbol esters seem to be responsible for tumor promoting activity. One element is formed of certain hyrophilic groups which are supposed to be responsible for the specific receptor binding. The other element consists of hydrophobic groups which should rather unspecifically be responsible for partition and transport between biological phases. In order to differentiate between these two structural elements, the numerical relative tumor promoting activity of phorbol diesters (a new activity in QSAR) was calculated from rodent skin painting experiments and its dependence from hydrophobicity was modeled using the parabolic and the bilinear model. The results show that the tumor promoting activity of aliphatic phorbol 12,13-diesters can adequately be described by hydrophobicity only. This indicates that the structural element 'aliphatic-12,13-diesters is rather unspecifically responsible for partition and transport between biological phases. A medium hydrophobicity caused by aliphatic ester chains in position 12 and 13 of phorbol is a sufficient condition for high promoting activity as long as the other hydrophilic groups are not removed, acylated or otherwise changed.

L4 ANSWER 24 OF 25 BIOSIS COPYRIGHT 2004 BIOLOGICAL ABSTRACTS INC. on STN
Full Text

AN 1987:329074 BIOSIS

DN PREV198733039671; BR33:39671

TI COMPARISON OF THE QUANTITATIVE DOSE-RESPONSE RELATIONSHIPS IN MOUSE SKIN OF SOLITARY CARCINOGENESIS AND INITIATION-PROMOTION A FIRST EXAMPLE BY 7 12 DIMETHYLBENZ-A-ANTHRACENE DMBA AND 3-O TETRADECANOYLINGENOL 3-TI.

AU **RIPPMANN F** [Reprint author]; ROESER H; HECKER E

CS GERMAN CANCER RES CENT, INST BIOCHEM, IM NEUENHEIMER FELD 280, D-6900 HEIDELBERG

SO Journal of Cancer Research and Clinical Oncology, (1987) Vol. 113, No. SUPPL, pp. S20.
Meeting Info.: FOURTH SYMPOSIUM OF THE DEUTSCHEN KREBSGESELLSCHAFT, SECTION EXPERIMENTELLE KREBSFORSCHUNG (GERMAN CANCER SOCIETY, SECTION OF EXPERIMENTAL CANCER RESEARCH), HEIDELBERG, WEST GERMANY, MARCH 18-21, 1987. J CANCER RES CLIN ONCOL.
CODEN: JCROD7. ISSN: 0171-5216.

DT Conference; (Meeting)

FS BR

LA ENGLISH

ED Entered STN: 25 Jul 1987
Last Updated on STN: 25 Jul 1987

L4 ANSWER 25 OF 25 BIOSIS COPYRIGHT 2004 BIOLOGICAL ABSTRACTS INC. on STN
Full Text

AN 1987:329058 BIOSIS

DN PREV198733039655; BR33:39655

TI QUANTITATIVE COMPARISON OF TUMORIGENICITY AND DNA BINDING BY 9 10 DIMETHYLANTHRACENE AND 7 12 DIMETHYLBENZ-A-ANTHRACENE.

AU FRIESEL H [Reprint author]; **RIPPMANN F**; SCHNEIDER T; SCHOEPE K-B; HECKER E

CS GERMAN CANCER RES CENT, INST BIOCHEM, IM NEUENHEIMER FELD 280, D-6900 HEIDELBERG

SO Journal of Cancer Research and Clinical Oncology, (1987) Vol. 113, No. SUPPL, pp. S16.
Meeting Info.: FOURTH SYMPOSIUM OF THE DEUTSCHEN KREBSGESELLSCHAFT, SECTION EXPERIMENTELLE KREBSFORSCHUNG (GERMAN CANCER SOCIETY, SECTION OF EXPERIMENTAL CANCER RESEARCH), HEIDELBERG, WEST GERMANY, MARCH 18-21,

1987. J CANCER RES CLIN ONCOL.
CODEN: JCROD7. ISSN: 0171-5216.
DT Conference; (Meeting)
FS BR
LA ENGLISH
ED Entered STN: 25 Jul 1987
Last Updated on STN: 25 Jul 1987

=> s sequence and search and (iterative or sequential)
L5 394 SEQUENCE AND SEARCH AND (ITERATIVE OR SEQUENTIAL)

=> s l5 and database
L6 150 L5 AND DATABASE

=> s l6 and (remov? or separat?)
L7 6 L6 AND (REMOV? OR SEPARAT?)

=> duplicate remove l7
DUPLICATE PREFERENCE IS 'MEDLINE, BIOSIS'
KEEP DUPLICATES FROM MORE THAN ONE FILE? Y/(N):n
PROCESSING COMPLETED FOR L7
L8 5 DUPLICATE REMOVE L7 (1 DUPLICATE REMOVED)

=> d 1-5 bib ab

L8 ANSWER 1 OF 5 MEDLINE on STN
Full Text
AN 2004119277 MEDLINE
DN PubMed ID: 15009210
TI The structure-function relationship in the clostripain family of peptidases.
AU Labrou Nikolaos E; Rigden Daniel J
CS Laboratory of Enzyme Technology, Department of Agricultural Biotechnology, Agricultural University of Athens, Greece.. Lambrou@aua.gr
SO European journal of biochemistry / FEBS, (2004 Mar) 271 (5) 983-92.
Journal code: 0107600. ISSN: 0014-2956.
CY Germany: Germany, Federal Republic of
DT Journal; Article; (JOURNAL ARTICLE)
LA English
FS Priority Journals
EM 200404
ED Entered STN: 20040311
Last Updated on STN: 20040408
Entered Medline: 20040407
AB In this study we investigate the active-site structure and the catalytic mechanism of clostripain by using a combination of three **separate** techniques: affinity labelling, site-directed mutagenesis and molecular modelling. A benzamidinyl-diazo dichlorotriazine dye (BDD) was shown to act as an efficient active site-directed affinity label for Clostridium histolyticum clostripain. The enzyme, upon incubation with BDD in 0.1 m Hepes/NaOH buffer pH 7.6, exhibits a time-dependent loss of activity. The rate of inactivation exhibits a nonlinear dependence on the BDD concentration, which can be described by reversible binding of dye to the enzyme prior to the irreversible reaction. The dissociation constant of the reversible formation of an enzyme-BDD complex is KD = 74.6 +/- 2.1 micro m and the maximal rate constant of inactivation is k3 = 0.21 x min(-1). Effective protection against inactivation by BDD is provided by the substrate N-benzoyl-L-arginine ethyl ester (BAEE). Cleavage of BDD-modified enzyme with trypsin and subsequent **separation** of peptides

by reverse-phase HPLC gave only one modified peptide. Amino acid sequencing of the modified tryptic peptide revealed the target site of BDD reaction to be His176. Site-directed mutagenesis was used to study further the functional role of His176. The mutant His176Ala enzyme exhibited zero activity against BAEE. Together with previous data, these results confirm that a catalytic dyad of His176 and Cys231 is responsible for cysteine peptidase activity in the C11 peptidase family. A molecular model of the catalytic domain of clostripain was constructed using a manually extended fold recognition-derived alignment with caspases. A rigorous **iterative** modelling scheme resulted in an objectively sound model which points to Asp229 as responsible for defining the strong substrate specificity for Arg at the P1 position. Two possible binding sites for the calcium required for auto-activation could be located. **Database searches** show that clostripain homologues are not confined to bacterial lineages and reveal an intriguing variety of domain architectures.

L8 ANSWER 2 OF 5 MEDLINE on STN
Full Text
AN 2004066366 MEDLINE
DN PubMed ID: 14729914
TI In-depth analysis of the thylakoid membrane proteome of Arabidopsis thaliana chloroplasts: new proteins, new functions, and a plastid proteome **database.**
AU Friso Giulia; Giacomelli Lisa; Ytterberg A Jimmy; Peltier Jean-Benoit; Rudella Andrea; Sun Qi; Wijk Klaas J van
CS Department of Plant Biology, Cornell University, Ithaca, New York 14853, USA.
SO Plant cell, (2004 Feb) 16 (2) 478-99.
Journal code: 9208688. ISSN: 1040-4651.
CY United States
DT Journal; Article; (JOURNAL ARTICLE)
LA English
FS Priority Journals
OS GENBANK-AL132972
EM 200406
ED Entered STN: 20040210
Last Updated on STN: 20040625
Entered Medline: 20040623
AB An extensive analysis of the Arabidopsis thaliana peripheral and integral thylakoid membrane proteome was performed by **sequential** extractions with salt, detergent, and organic solvents, followed by multidimensional protein **separation** steps (reverse-phase HPLC and one- and two-dimensional electrophoresis gels), different enzymatic and nonenzymatic protein cleavage techniques, mass spectrometry, and bioinformatics. Altogether, 154 proteins were identified, of which 76 (49%) were alpha-helical integral membrane proteins. Twenty-seven new proteins without known function but with predicted chloroplast transit peptides were identified, of which 17 (63%) are integral membrane proteins. These new proteins, likely important in thylakoid biogenesis, include two rubredoxins, a potential metallochaperone, and a new DnaJ-like protein. The data were integrated with our analysis of the lumenal-enriched proteome. We identified 83 out of 100 known proteins of the thylakoid localized photosynthetic apparatus, including several new paralogues and some 20 proteins involved in protein insertion, assembly, folding, or proteolysis. An additional 16 proteins are involved in translation, demonstrating that the thylakoid membrane surface is an important site for protein synthesis. The high coverage of the photosynthetic apparatus and the identification of known hydrophobic proteins with low expression levels, such as cpSecE, Ohp1, and Ohp2,

indicate an excellent dynamic resolution of the analysis. The **sequential** extraction process proved very helpful to validate transmembrane prediction. Our data also were cross-correlated to chloroplast subproteome analyses by other laboratories. All data are deposited in a new curated plastid proteome **database** (PPDB) with multiple **search** functions (http://cbsusrv01.tc.cornell.edu/users/ppdb/). This PPDB will serve as an expandable resource for the plant community.

L8 ANSWER 3 OF 5 MEDLINE on STN DUPLICATE 1
Full Text
AN 2003297400 IN-PROCESS
DN PubMed ID: 12824488
TI Three monophyletic superfamilies account for the majority of the known glycosyltransferases.
AU Liu Jing; Mushegian Arcady
CS Stowers Institute for Medical Research, 1000 E. 50th Street, Kansas City, MO 64110, USA.
SO Protein science : a publication of the Protein Society, (2003 Jul) 12 (7) 1418-31.
Journal code: 9211750. ISSN: 0961-8368.
CY United States
DT Journal; Article; (JOURNAL ARTICLE)
LA English
FS IN-PROCESS; NONINDEXED; Priority Journals
ED Entered STN: 20030626
Last Updated on STN: 20031218
AB Sixty-five families of glycosyltransferases (EC 2.4.x.y) have been recognized on the basis of high-**sequence** similarity to a founding member with experimentally demonstrated enzymatic activity. Although distant **sequence** relationships between some of these families have been reported, the natural history of glycosyltransferases is poorly understood. We used **iterative searches** of **sequence databases,** motif extraction, structural comparison, and analysis of completely sequenced genomes to track the origins of modern-type glycosyltransferases. We show that >75% of recognized glycosyltransferase families belong to one of only three monophyletic superfamilies of proteins, namely, (1) a recently described GPGTF/GT-B superfamily; (2) a nucleoside-diphosphosugar transferase (GT-A) superfamily, which is characterized by a DxD **sequence** signature and also includes nucleotidyltransferases; and (3) a GT-C superfamily of integral membrane glycosyltransferases with a modified DxD signature in the first extracellular loop. Several developmental regulators in Metazoans, including Fringe and Egghead homologs, belong to the second superfamily. Interestingly, Tout-velu/Exostosin family of developmental proteins found in all multicellular eukaryotes, contains **separate** domains belonging to the first and the second superfamilies, explaining multiple glycosyltransferase activities in one protein.

L8 ANSWER 4 OF 5 MEDLINE on STN
Full Text
AN 2001700727 MEDLINE
DN PubMed ID: 11741263
TI Evolutionary relationships among G protein-coupled receptors using a clustered **database** approach.
AU Graul R C; Sadee W
CS Incyte Genomics, Palo Alto, CA 94304, USA.
NC GM43102 (NIGMS)
SO AAPS pharmSci [electronic resource], (2001) 3 (2) E12.
Journal code: 100897065. ISSN: 1522-1059.
CY United States

DT Journal; Article; (JOURNAL ARTICLE)
LA English
FS Priority Journals
EM 200202
ED Entered STN: 20011220
Last Updated on STN: 20020212
Entered Medline: 20020211
AB Guanine nucleotide-binding protein-coupled receptors (GPCRs) comprise large and diverse gene families in fungi, plants, and the animal kingdom. GPCRs appear to share a common structure with 7 transmembrane segments, but **sequence** similarity is minimal among the most distant GPCRs. To reevaluate the question of evolutionary relationships among the disparate GPCR families, this study takes advantage of the dramatically increased number of cloned GPCRs. **Sequences** were selected from the National Center for Biotechnology Information (NCBI) nonredundant peptide **database** using **iterative** BLAST (Basic Local Alignment **Search** Tool) **searches** to yield a **database** of approximately 1700 GPCRs and unrelated membrane proteins as controls, divided into 34 distinct clusters. For each cluster, **separate** position-specific matrices were established to optimize **sequence** comparisons among GPCRs. This approach resulted in significant alignments between distant GPCR families, including receptors for the biogenic amine/peptide, VIP/secretin, cAMP, STE3/MAP3 fungal pheromones, latrophilin, developmental receptors frizzled and smoothened, as well as the more distant metabotrobic glutamate receptors, the STE2/MAM2 fungal pheromone receptors, and GPR1, a fungal glucose receptor. On the other hand, alignment scores between these recognized GPCR clades with p40 (putative GPCR) and pm1 (putative GPCR), as well as bacteriorhodopsins, failed to support a finding of homology. This study provides a refined view of GPCR ancestry and serves as a reference **database** with hyperlinks to other sources. Moreover, it may facilitate **database** annotation and the assignment of orphan receptors to GPCR families.

L8 ANSWER 5 OF 5 BIOSIS COPYRIGHT 2004 BIOLOGICAL ABSTRACTS INC. on STN
Full Text
AN 2000:375555 BIOSIS
DN PREV200000375555
TI Homology-based method for identification of protein repeats using statistical significance estimates.
AU Andrade, Miguel A.; Ponting, Chris P.; Gibson, Toby J.; Bork, Peer [Reprint author]
CS European Molecular Biology Laboratory, Meyerhofstr. 1, Heidelberg, 69012, Germany
SO Journal of Molecular Biology, (May 5, 2000) Vol. 298, No. 3, pp. 521-537. print.
CODEN: JMOBAK. ISSN: 0022-2836.
DT Article
LA English
ED Entered STN: 6 Sep 2000
Last Updated on STN: 8 Jan 2002
AB Short protein repeats, frequently with a length between 20 and 40 residues, represent a significant fraction of known proteins. Many repeats appear to possess high amino acid substitution rates and thus recognition of repeat homologues is highly problematic. Even if the presence of a certain repeat family is known, the exact locations and the number of repetitive units often cannot be determined using current methods. We have devised an **iterative** algorithm based on optimal and sub-optimal score distributions from profile analysis that estimates the significance of all repeats that are detected in a single **sequence.** This procedure allows the identification of homologues at alignment scores

lower than the highest optimal alignment score for non-homologous **sequences**. The method has been used to investigate the occurrence of eleven families of repeats in Saccharomyces cerevisiae, Caenorhabditis elegans and Homo sapiens accounting for 1055, 2205 and 2320 repeats, respectively. For these examples, the method is both more sensitive and more selective than conventional homology **search** procedures. The method allowed the detection in the SwissProt **database** of more than 2000 previously unrecognised repeats belonging to the 11 families. In addition, the method was used to merge several repeat families that previously were supposed to be distinct, indicating common phylogenetic origins for these families.

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L1          21 S E3-6
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L3          32 S E15-16
L4          25 DUPLICATE REMOVE L3 (7 DUPLICATES REMOVED)
L5         394 S SEQUENCE AND SEARCH AND (ITERATIVE OR SEQUENTIAL)
L6         150 S L5 AND DATABASE
L7           6 S L6 AND (REMOV? OR SEPARAT?)
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L9          46 L6 AND (SOFTWARE OR PROGRAM)

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L10         29 DUPLICATE REMOVE L9 (17 DUPLICATES REMOVED)

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L10  ANSWER 1 OF 29  BIOSIS  COPYRIGHT 2004 BIOLOGICAL ABSTRACTS INC. on STN
Full Text
AN   2003:135603  BIOSIS
DN   PREV200300135603
TI   Search for structural similarity in proteins.
AU   Leluk, Jacek; Konieczny, Leszek; Roterman, Irena [Reprint Author]
CS   Department of Biostatistics and Medical Informatics, Collegium Medicum,
     Jagiellonian University, Kopernika 17, 31-501, Krakow, Poland
     lulu@bf.uni.wroc.pl; myroterm@cyf-kr.edu.pl
SO   Bioinformatics (Oxford), (January 2003) Vol. 19, No. 1, pp. 117-124.
     print.
     ISSN: 1367-4803.
DT   Article
LA   English
ED   Entered STN: 12 Mar 2003
     Last Updated on STN: 12 Mar 2003
AB   Motivation: The expanding protein sequence and structure databases
     await methods allowing rapid similarity search. Geometric
     parameters-dihedral angle between two sequential peptide bond planes (V)
     and radius of curvature (R) as they appear in pentapeptide fragments in
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polypeptide chains-are proposed for use in evaluating structural similarity in proteins (VeaR). The parabolic (empirical) function expressing the radius of curvature's dependence on the V-angle in model polypeptides is altered in real proteins in a form characteristic for a particular protein. This can be used as a criterion for judging similarity. Results: A structural comparison of proteins representing a wide spectrum of structures was assessed versus **sequence** similarity analysis based on the genetic semihomology algorithm. The term 'consensus structure', analogous to 'consensus **sequence**', was introduced for the serpine family.

L10 ANSWER 2 OF 29 MEDLINE on STN
Full Text
AN 2003243846 MEDLINE
DN PubMed ID: 12766406
TI PACES: Protein **sequential** assignment by computer-assisted exhaustive **search**.
AU Coggins Brian E; Zhou Pei
CS Department of Biochemistry, Duke University Medical Center, Durham, NC 27710, U.S.A.
NC GM 51310 (NIGMS)
SO Journal of biomolecular NMR, (2003 Jun) 26 (2) 93-111.
Journal code: 9110829. ISSN: 0925-2738.
CY Netherlands
DT (EVALUATION STUDIES)
Journal; Article; (JOURNAL ARTICLE)
LA English
FS Priority Journals
EM 200403
ED Entered STN: 20030528
Last Updated on STN: 20040305
Entered Medline: 20040304
AB A crucial step in determining solution structures of proteins using nuclear magnetic resonance (NMR) spectroscopy is the process of **sequential** assignment, which correlates backbone resonances to corresponding residues in the primary **sequence** of a protein, today, typically using data from triple-resonance NMR experiments. Although the development of automated approaches for **sequential** assignment has greatly facilitated this process, the performance of these **programs** is usually less satisfactory for large proteins, especially in the cases of missing connectivity or severe chemical shift degeneracy. Here, we report the development of a novel computer-assisted method for **sequential** assignment, using an algorithm that conducts an exhaustive **search** of all spin systems both for establishing **sequential** connectivities and then for assignment. By running the **program** iteratively with user intervention after each cycle, ambiguities in the assignments can be eliminated efficiently and backbone resonances can be assigned rapidly. The efficiency and robustness of this approach have been tested with 27 proteins of sizes varying from 76 amino acids to 723 amino acids, and with data of varying qualities, using experimental data for three proteins, and published assignments modified with simulated noise for the other 24. The complexity of **sequential** assignment with regard to the size of the protein, the completeness of NMR data sets, and the uncertainty in resonance positions has been examined.

L10 ANSWER 3 OF 29 MEDLINE on STN DUPLICATE 1
Full Text
AN 2002609982 MEDLINE
DN PubMed ID: 12364612
TI A comparison of profile hidden Markov model procedures for remote homology

detection.
AU Madera Martin; Gough Julian
CS MRC Laboratory of Molecular Biology, Hills Road, Cambridge CB2 2QH, UK.. mm238@mrc-lmb.cam.ac.uk
SO Nucleic acids research, (2002 Oct 1) 30 (19) 4321-8.
Journal code: 0411011. ISSN: 1362-4962.
CY England: United Kingdom
DT Journal; Article; (JOURNAL ARTICLE)
LA English
FS Priority Journals
EM 200212
ED Entered STN: 20021008
Last Updated on STN: 20021218
Entered Medline: 20021216
AB Profile hidden Markov models (HMMs) are amongst the most successful procedures for detecting remote homology between proteins. There are two popular profile HMM **programs**, HMMER and SAM. Little is known about their performance relative to each other and to the recently improved version of PSI-BLAST. Here we compare the two **programs** to each other and to non-HMM methods, to determine their relative performance and the features that are important for their success. The quality of the multiple **sequence** alignments used to build models was the most important factor affecting the overall performance of profile HMMs. The SAM T99 procedure is needed to produce high quality alignments automatically, and the lack of an equivalent component in HMMER makes it less complete as a package. Using the default options and parameters as would be expected of an inexpert user, it was found that from identical alignments SAM consistently produces better models than HMMER and that the relative performance of the model-scoring components varies. On average, HMMER was found to be between one and three times faster than SAM when searching **databases** larger than 2000 **sequences**, SAM being faster on smaller ones. Both methods were shown to have effective low complexity and repeat **sequence** masking using their null models, and the accuracy of their E-values was comparable. It was found that the SAM T99 **iterative database search** procedure performs better than the most recent version of PSI-BLAST, but that scoring of PSI-BLAST profiles is more than 30 times faster than scoring of SAM models.

L10 ANSWER 4 OF 29 MEDLINE on STN
Full Text
AN 2002327708 MEDLINE
DN PubMed ID: 12070318
TI The family of toxin-related ecto-ADP-ribosyltransferases in humans and the mouse.
AU Glowacki Gustavo; Braren Rickmer; Firner Kathrin; Nissen Marion; Kuhl Maren; Reche Pedro; Bazan Fernando; Cetkovic-Cvrlje Marina; Leiter Edward; Haag Friedrich; Koch-Nolte Friedrich
CS Institute of Immunology, University Hospital, Martinistrasse 52, D-20246 Hamburg, Germany.
NC DK 27722 (NIDDK)
DK 36173 (NIDDK)
SO Protein science : a publication of the Protein Society, (2002 Jul) 11 (7) 1657-70.
Journal code: 9211750. ISSN: 0961-8368.
CY United States
DT Journal; Article; (JOURNAL ARTICLE)
LA English
FS Priority Journals
EM 200308
ED Entered STN: 20020619

Last Updated on STN: 20021211
Entered Medline: 20030819

AB ADP-ribosyltransferases including toxins secreted by Vibrio cholera, Pseudomonas aerurginosa, and other pathogenic bacteria inactivate the function of human target proteins by attaching ADP-ribose onto a critical amino acid residue. Cross-species polymerase chain reaction (PCR) and **database** mining identified the orthologs of these ADP-ribosylating toxins in humans and the mouse. The human genome contains four functional toxin-related ADP-ribosyltransferase genes (ARTs) and two related intron-containing pseudogenes; the mouse has six functional orthologs. The human and mouse ART genes map to chromosomal regions with conserved linkage synteny. The individual ART genes reveal highly restricted expression patterns, which are largely conserved in humans and the mouse. We confirmed the predicted extracellular location of the ART proteins by expressing recombinant ARTs in insect cells. Two human and four mouse ARTs contain the active site motif (R-S-EXE) typical of arginine-specific ADP-ribosyltransferases and exhibit the predicted enzyme activities. Two other human ARTs and their murine orthologues deviate in the active site motif and lack detectable enzyme activity. Conceivably, these ARTs may have acquired a new specificity or function. The position-sensitive **iterative database search program** PSI-BLAST connected the mammalian ARTs with most known bacterial ADP-ribosylating toxins. In contrast, no related open reading frames occur in the four completed genomes of lower eucaryotes (yeast, worm, fly, and mustard weed). Interestingly, these organisms also lack genes for ADP-ribosylhydrolases, the enzymes that reverse protein ADP-ribosylation. This suggests that the two enzyme families that catalyze reversible mono-ADP-ribosylation either were lost from the genomes of these nonchordata eucaryotes or were subject to horizontal gene transfer between kingdoms.

L10 ANSWER 5 OF 29 MEDLINE on STN DUPLICATE 2
Full Text
AN 2002610661 MEDLINE
DN PubMed ID: 12368255
TI CDART: protein homology by domain architecture.
AU Geer Lewis Y; Domrachev Michael; Lipman David J; Bryant Stephen H
CS National Center for Biotechnology Information, National Library of Medicine, National Institutes of Health, Bethesda, Maryland 20894, USA.. lewisg@mail.nih.gov
SO Genome research, (2002 Oct) 12 (10) 1619-23.
Journal code: 9518021. ISSN: 1088-9051.
CY United States
DT Journal; Article; (JOURNAL ARTICLE)
LA English
FS Priority Journals
EM 200304
ED Entered STN: 20021008
Last Updated on STN: 20030416
Entered Medline: 20030411

AB The Conserved Domain Architecture Retrieval Tool (CDART) performs similarity **searches** of the NCBI Entrez Protein **Database** based on domain architecture, defined as the **sequential** order of conserved domains in proteins. The algorithm finds protein similarities across significant evolutionary distances using sensitive protein domain profiles rather than by direct **sequence** similarity. Proteins similar to a query protein are grouped and scored by architecture. Relying on domain profiles allows CDART to be fast, and, because it relies on annotated functional domains, informative. Domain profiles are derived from several collections of domain definitions that include functional annotation. **Searches** can be further refined by taxonomy and by selecting domains of

interest. CDART is available at http://www.ncbi.nlm.nih.gov/Structure/lexington/lexington.cgi.

L10 ANSWER 6 OF 29 MEDLINE on STN DUPLICATE 3
Full Text
AN 2002618987 MEDLINE
DN PubMed ID: 12376380
TI Data mining of **sequences** and 3D structures of allergenic proteins.
AU Ivanciuc Ovidiu; Schein Catherine H; Braun Werner
CS Sealy Center for Structural Biology, Department of Human Biological Chemistry and Genetics, University of Texas Medical Branch, Galveston, TX 77555-1157, USA.
SO Bioinformatics (Oxford, England), (2002 Oct) 18 (10) 1358-64.
Journal code: 9808944. ISSN: 1367-4803.
CY England: United Kingdom
DT Journal; Article; (JOURNAL ARTICLE)
LA English
FS Priority Journals
EM 200304
ED Entered STN: 20021012
Last Updated on STN: 20030501
Entered Medline: 20030430
AB MOTIVATION: Many **sequences**, and in some cases structures, of proteins that induce an allergic response in atopic individuals have been determined in recent years. This data indicates that allergens, regardless of source, fall into discreet protein families. Similarities in the **sequence** may explain clinically observed cross-reactivities between different biological triggers. However, previously available allergy **databases** group allergens according to their biological sources, or observed clinical cross-reactivities, without providing data about the proteins. A computer-aided data mining system is needed to compare the **sequential** and structural details of known allergens. This information will aid in predicting allergenic cross-responses and eventually in determining possible common characteristics of IgE recognition. RESULTS: The new web-based Structural **Database** of Allergenic Proteins (SDAP) permits the user to quickly compare the **sequence** and structure of allergenic proteins. Data from literature sources and previously existing lists of allergens are combined in a MySQL interactive **database** with a wide selection of bioinformatics applications. SDAP can be used to rapidly determine the relationship between allergens and to screen novel proteins for the presence of IgE or T-cell epitopes they may share with known allergens. Further, our novel similarity **search** method, based on five dimensional descriptors of amino acid properties, can be used to scan the SDAP entries with a peptide **sequence**. For example, when a known IgE binding epitope from shrimp tropomyosin was used as a query, the method rapidly identified a similar **sequence** in known shellfish and insect allergens. This prediction of cross-reactivity between allergens is consistent with clinical observations. AVAILABILITY: SDAP is available on the web at http://fermi.utmb.edu/SDAP/index.html

L10 ANSWER 7 OF 29 MEDLINE on STN DUPLICATE 4
Full Text
AN 2002696672 MEDLINE
DN PubMed ID: 12458087
TI A survey of metazoan selenocysteine insertion **sequences**.
AU Lambert Andre; Lescure Alain; Gautheret Daniel
CS CNRS UPR 7061, Marseille, France.
SO Biochimie, (2002 Sep) 84 (9) 953-9.
Journal code: 1264604. ISSN: 0300-9084.
CY France

DT Journal; Article; (JOURNAL ARTICLE)
LA English
FS Priority Journals
EM 200306
ED Entered STN: 20021217
Last Updated on STN: 20030611
Entered Medline: 20030610
AB The computational detection of novel selenoproteins in genomic **sequences** is usually achieved through identification of SECIS, a conserved secondary structure element found in the 3' UTR of animal selenoprotein mRNAs. Previous studies have used "descriptors" specifying the number of base pairs and the conserved nucleotides in SECIS to identify this element. A major drawback of the "descriptor" approach is that the number of detections in current genomic or transcript **databases** largely exceeds the number of true selenoproteins. In this study, we use instead the ERPIN **program** to detect SECIS elements. ERPIN is based on a lod-score profile algorithm that uses a training-set of aligned RNA **sequences** as input. From an initial alignment of 44 animal SECIS **sequences**, we performed a series of **iterative searches** in which the training set was progressively enriched up to 117 confirmed SECIS elements, from a large collection of metazoan species. About 200 high-scoring candidates were also detected. We show that ERPIN scores for these candidates can be converted into expect values, thus enabling their statistical evaluation. The most interesting SECIS candidates are presented.

L10 ANSWER 8 OF 29 MEDLINE on STN DUPLICATE 5
Full Text
AN 2002004331 MEDLINE
DN PubMed ID: 11752353
TI RIDOM: Ribosomal Differentiation of Medical Micro-organisms **Database**.
AU Harmsen Dag; Rothganger Jorg; Frosch Matthias; Albert Jurgen
CS Institut fur Hygiene und Mikrobiologie, Universitat Wurzburg, D-97080 Wurzburg, Germany.. dharmsen@ridom.de
SO Nucleic acids research, (2002 Jan 1) 30 (1) 416-7.
Journal code: 0411011. ISSN: 1362-4962.
CY England: United Kingdom
DT Journal; Article; (JOURNAL ARTICLE)
LA English
FS Priority Journals
EM 200201
ED Entered STN: 20020102
Last Updated on STN: 20020125
Entered Medline: 20020121
AB The ribosomal differentiation of medical micro-organisms (RIDOM) web server, first described by Harmsen et al. [Harmsden,D., Rothganger,J., Singer,C., Albert,J. and Frosch,M. (1999) Lancet, 353, 291], is an evolving electronic resource designed to provide micro-organism differentiation services for medical identification needs. The diagnostic procedure begins with a specimen partial small subunit ribosomal DNA (16S rDNA) **sequence**. Resulting from a similarity **search**, a species or genus name for the specimen in question will be returned. Where the first results are ambiguous or do not define to species level, hints for further molecular, i.e. internal transcribed spacer, and conventional phenotypic differentiation will be offered ('**sequential** and polyphasic approach'). Additionally, each entry in RIDOM contains detailed medical and taxonomic information linked, context-sensitive, to external World Wide Web services. Nearly all **sequences** are newly determined and the **sequence** chromatograms are available for intersubjective quality control. Similarity **searches** are now also possible by direct submission of trace files (ABI or SCF format). Based on the PHRED/PHRAP **software**, error

probability measures are attached to each predicted nucleotide base and visualised with a new 'Trace Editor'. The RIDOM web site is directly accessible on the World Wide Web at http://www.ridom.de/. The email address for questions and comments is webmaster@ridom.de.

L10 ANSWER 9 OF 29 MEDLINE on STN DUPLICATE 6
Full Text
AN 2001400776 MEDLINE
DN PubMed ID: 11452024
TI Improving the accuracy of PSI-BLAST protein **database searches** with composition-based statistics and other refinements.
AU Schaffer A A; Aravind L; Madden T L; Shavirin S; Spouge J L; Wolf Y I; Koonin E V; Altschul S F
CS National Center for Biotechnology Information, National Institutes of Health, 8600 Rockville Pike, Bethesda, MD 20894, USA.. schaffer@helix.nih.gov
SO Nucleic acids research, (2001 Jul 15) 29 (14) 2994-3005. Ref: 60
Journal code: 0411011. ISSN: 1362-4962.
CY England: United Kingdom
DT Journal; Article; (JOURNAL ARTICLE)
General Review; (REVIEW)
(REVIEW, TUTORIAL)
LA English
FS Priority Journals
EM 200109
ED Entered STN: 20010910
Last Updated on STN: 20010910
Entered Medline: 20010906
AB PSI-BLAST is an **iterative program** to **search** a **database** for proteins with distant similarity to a query **sequence**. We investigated over a dozen modifications to the methods used in PSI-BLAST, with the goal of improving accuracy in finding true positive matches. To evaluate performance we used a set of 103 queries for which the true positives in yeast had been annotated by human experts, and a popular measure of retrieval accuracy (ROC) that can be normalized to take on values between 0 (worst) and 1 (best). The modifications we consider novel improve the ROC score from 0.758 +/- 0.005 to 0.895 +/- 0.003. This does not include the benefits from four modifications we included in the 'baseline' version, even though they were not implemented in PSI-BLAST version 2.0. The improvement in accuracy was confirmed on a small second test set. This test involved analyzing three protein families with curated lists of true positives from the non-redundant protein **database**. The modification that accounts for the majority of the improvement is the use, for each **database sequence**, of a position-specific scoring system tuned to that **sequence**'s amino acid composition. The use of composition-based statistics is particularly beneficial for large-scale automated applications of PSI-BLAST.

L10 ANSWER 10 OF 29 MEDLINE on STN DUPLICATE 7
Full Text
AN 2001647953 MEDLINE
DN PubMed ID: 11700055
TI Direct RNA motif definition and identification from multiple **sequence** alignments using secondary structure profiles.
AU Gautheret D; Lambert A
CS Centre d'Immunologie de Marseille Luminy, CNRS UMR 6102/INSERM U 136, Luminy Case 906, 13288 Marseille Cedex 09, France.. gautheret@esil.univ-mrs.fr
SO Journal of molecular biology, (2001 Nov 9) 313 (5) 1003-11.
Journal code: 2985088R. ISSN: 0022-2836.

CY England: United Kingdom
DT Journal; Article; (JOURNAL ARTICLE)
LA English
FS Priority Journals
EM 200112
ED Entered STN: 20011112
Last Updated on STN: 20020123
Entered Medline: 20011207
AB We present here a new approach to the problem of defining RNA signatures and finding their occurrences in **sequence databases**. The proposed method is based on "secondary structure profiles". An RNA **sequence** alignment with secondary structure information is used as an input. Two types of weight matrices/profiles are constructed from this alignment: single strands are represented by a classical lod-scores profile while helical regions are represented by an extended "helical profile" comprising 16 lod-scores per position, one for each of the 16 possible base-pairs. **Database searches** are then conducted using a simultaneous **search** for helical profiles and dynamic programming alignment of single strand profiles. The algorithm has been implemented into a new **software**, ERPIN, that performs both profile construction and **database search**. Applications are presented for several RNA motifs. The automated use of **sequence** information in both single-stranded and helical regions yields better sensitivity/specificity ratios than descriptor-based **programs**. Furthermore, since the translation of alignments into profiles is straightforward with ERPIN, **iterative searches** can easily be conducted to enrich collections of homologous RNAs. Copyright 2001 Academic Press.

L10 ANSWER 11 OF 29 MEDLINE on STN
Full Text
AN 2001480902 MEDLINE
DN PubMed ID: 11524372
TI Evaluation of protein multiple alignments by SAM-T99 using the BAliBASE multiple alignment test set.
AU Karplus K; Hu B
CS Computer Engineering, University of California, Santa Cruz, 59064, USA.
SO Bioinformatics (Oxford, England), (2001 Aug) 17 (8) 713-20.
Journal code: 9808944. ISSN: 1367-4803.
CY England: United Kingdom
DT (EVALUATION STUDIES)
Journal; Article; (JOURNAL ARTICLE)
LA English
FS Priority Journals
EM 200112
ED Entered STN: 20010830
Last Updated on STN: 20020122
Entered Medline: 20011204
AB MOTIVATION: SAM-T99 is an **iterative** hidden Markov model-based method for finding proteins similar to a single target **sequence** and aligning them. One of its main uses is to produce multiple alignments of homologs of the target **sequence**. Previous tests of SAM-T99 and its predecessors have concentrated on the quality of the **searches** performed, not on the quality of the multiple alignment. In this paper we report on tests of multiple alignment quality, comparing SAM-T99 to the standard multiple aligner, CLUSTALW. RESULTS: The paper evaluates the multiple-alignment aspect of the SAM-T99 protocol, using the BAliBASE benchmark alignment **database**. On these benchmarks, SAM-T99 is comparable in accuracy with ClustalW. AVAILABILITY: The SAM-T99 protocol can be run on the web at http://www.cse.ucsc.edu/research/compbio/HMM-apps/T99-query.html and the alignment tune-up option described here can be run at

http://www.cse.ucsc.edu/research/compbio/HMM-apps/T99-tuneup.html. The protocol is also part of the standard SAM suite of tools. http://www.cse.ucsc.edu/research/compbio/sam/

L10 ANSWER 12 OF 29 MEDLINE on STN DUPLICATE 8
Full Text
AN 2001610257 MEDLINE
DN PubMed ID: 11684083
TI In silico analysis of the tRNA:m1A58 methyltransferase family: homology-based fold prediction and identification of new members from Eubacteria and Archaea.
AU Bujnicki J M
CS Bioinformatics Laboratory, International Institute of Molecular and Cell Biology, ul. ks. Trojdena 4, 02-109 Warsaw, Poland.. info@bioinfo.pl
SO FEBS letters, (2001 Oct 26) 507 (2) 123-7.
Journal code: 0155157. ISSN: 0014-5793.
CY Netherlands
DT Journal; Article; (JOURNAL ARTICLE)
LA English
FS Priority Journals
EM 200112
ED Entered STN: 20011102
Last Updated on STN: 20020123
Entered Medline: 20011211
AB The amino acid **sequences** of Gcd10p and Gcd14p, the two subunits of the tRNA:(1-methyladenosine-58; m(1)A58) methyltransferase (MTase) of Saccharomyces cerevisiae, have been analyzed using **iterative sequence database searches** and fold recognition **programs**. The results suggest that the 'catalytic' Gcd14p and 'substrate binding' Gcd10p are related to each other and to a group of prokaryotic open reading frames, which were previously annotated as hypothetical protein isoaspartate MTases in **sequence databases**. It is predicted that the prokaryotic proteins are genuine tRNA:m(1)A MTases based on similarity of their predicted active site to the Gcd14p family. In addition to the MTase domain, an additional domain was identified in the N-terminus of all these proteins that may be involved in interaction with tRNA. These results suggest that the eukaryotic tRNA:m(1)A58 MTase is a product of gene duplication and divergent evolution of a possibly homodimeric prokaryotic enzyme.

L10 ANSWER 13 OF 29 MEDLINE on STN DUPLICATE 9
Full Text
AN 2001336330 MEDLINE
DN PubMed ID: 11403999
TI Multiple alignment of complete **sequences** (MACS) in the post-genomic era.
AU Lecompte O; Thompson J D; Plewniak F; Thierry J; Poch O
CS Laboratoire de Biologie et Genomique Structurales, Institut de Genetique et de Biologie Moleculaire et Cellulaire (CNRS/INSERM/ULP), BP 163, 67404 Cedex, Illkirch, France.
SO Gene, (2001 May 30) 270 (1-2) 17-30. Ref: 137
Journal code: 7706761. ISSN: 0378-1119.
CY Netherlands
DT Journal; Article; (JOURNAL ARTICLE)
General Review; (REVIEW)
(REVIEW, TUTORIAL)
LA English
FS Priority Journals
EM 200108
ED Entered STN: 20010806
Last Updated on STN: 20010806

Entered Medline: 20010802

AB Multiple alignment, since its introduction in the early seventies, has become a cornerstone of modern molecular biology. It has traditionally been used to deduce structure / function by homology, to detect conserved motifs and in phylogenetic studies. There has recently been some renewed interest in the development of multiple alignment techniques, with current opinion moving away from a single all-encompassing algorithm to **iterative** and / or co-operative strategies. The exploitation of multiple alignments in genome annotation projects represents a qualitative leap in the functional analysis process, opening the way to the study of the co-evolution of validated sets of proteins and to reliable phylogenomic analysis. However, the alignment of the highly complex proteins detected by today's advanced **database search** methods is a daunting task. In addition, with the explosion of the **sequence databases** and with the establishment of numerous specialized biological **databases**, multiple alignment **programs** must evolve if they are to successfully rise to the new challenges of the post-genomic era. The way forward is clearly an integrated system bringing together **sequence** data, knowledge-based systems and prediction methods with their inherent unreliability. The incorporation of such heterogeneous, often non-consistent, data will require major changes to the fundamental alignment algorithms used to date. Such an integrated multiple alignment system will provide an ideal workbench for the validation, propagation and presentation of this information in a format that is concise, clear and intuitive.

L10 ANSWER 14 OF 29 BIOSIS COPYRIGHT 2004 BIOLOGICAL ABSTRACTS INC. on STN
Full Text

AN 2001:94236 BIOSIS

DN PREV200100094236

TI Evaluation of PSI-BLAST alignment accuracy in comparison to structural alignments.

AU Friedberg, Iddo; Kaplan, Tommy; Margalit, Hanah [Reprint author]

CS Department of Molecular Genetics and Biotechnology, The Hebrew University, Hadassah Medical School, Jerusalem, 91120, Israel
hanah@md2.huji.ac.il

SO Protein Science, (November, 2000) Vol. 9, No. 11, pp. 2278-2284. print.
ISSN: 0961-8368.

DT Article

LA English

ED Entered STN: 21 Feb 2001
Last Updated on STN: 12 Feb 2002

AB The PSI-BLAST algorithm has been acknowledged as one of the most powerful tools for detecting remote evolutionary relationships by **sequence** considerations only. This has been demonstrated by its ability to recognize remote structural homologues and by the greatest coverage it enables in annotation of a complete genome. Although recognizing the correct fold of a **sequence** is of major importance, the accuracy of the alignment is crucial for the success of modeling one **sequence** by the structure of its remote homologue. Here we assess the accuracy of PSI-BLAST alignments on a stringent **database** of 123 structurally similar, **sequence**-dissimilar pairs of proteins, by comparing them to the alignments defined on a structural basis. Each protein **sequence** is compared to a nonredundant **database** of the protein **sequences** by PSI-BLAST. Whenever a pair member detects its pair-mate, the positions that are aligned both in the **sequential** and structural alignments are determined, and the alignment sensitivity is expressed as the percentage of these positions out of the structural alignment. Fifty-two **sequences** detected their pair-mates (for 16 pairs the success was bi-directional when either pair member was used as a query). The average percentage of

correctly aligned residues per structural alignment was 43.5 +- 2.2%. Other properties of the alignments were also examined, such as the sensitivity vs. specificity and the change in these parameters over consecutive iterations. Notably, there is an improvement in alignment sensitivity over consecutive iterations, reaching an average of 50.9 +- 2.5% within the five iterations tested in the current study.

L10 ANSWER 15 OF 29 MEDLINE on STN DUPLICATE 10
Full Text
AN 2001027874 MEDLINE
DN PubMed ID: 10972829
TI The spvB gene-product of the Salmonella enterica virulence plasmid is a mono(ADP-ribosyl)transferase.
AU Otto H; Tezcan-Merdol D; Girisch R; Haag F; Rhen M; Koch-Nolte F
CS Institute for Immunology, University Hospital, Martinistr. 52, D-20246 Hamburg, Germany.
SO Molecular microbiology, (2000 Sep) 37 (5) 1106-15.
Journal code: 8712028. ISSN: 0950-382X.
CY ENGLAND: United Kingdom
DT Journal; Article; (JOURNAL ARTICLE)
LA English
FS Priority Journals
EM 200011
ED Entered STN: 20010322
Last Updated on STN: 20020420
Entered Medline: 20001115
AB A number of well-known bacterial toxins ADP-ribosylate and thereby inactivate target proteins in their animal hosts. Recently, several vertebrate ecto-enzymes (ART1-ART7) with activities similar to bacterial toxins have also been cloned. We show here that PSIBLAST, a position-specific-**iterative database search program**, faithfully connects all known vertebrate ecto-mono(ADP-ribosyl)transferases (mADPRTs) with most of the known bacterial mADPRTs. Intriguingly, no matches were found in the available public genome **sequences** of archaeabacteria, the yeast Saccharomyces cerevisiae or the nematode Caenorhabditis elegans. Significant new matches detected by PSIBLAST from the public **sequence** data bases included only one open reading frame (ORF) of previously unknown function: the spvB gene contained in the virulence plasmids of Salmonella enterica. Structure predictions of SpvB indicated that it is composed of a C-terminal ADP-ribosyltransferase domain fused via a poly proline stretch to a N-domain resembling the N-domain of the secretory toxin TcaC from nematode-infecting enterobacteria. We produced the predicted catalytic domain of SpvB as a recombinant fusion protein and demonstrate that it, indeed, acts as an ADP-ribosyltransferase. Our findings underscore the power of the PSIBLAST **program** for the discovery of new family members in genome **databases**. Moreover, they open a new avenue of investigation regarding salmonella pathogenesis.

L10 ANSWER 16 OF 29 MEDLINE on STN
Full Text
AN 2001211859 MEDLINE
DN PubMed ID: 11159310
TI **Iterative sequence**/secondary structure **search** for protein homologs: comparison with amino acid **sequence** alignments and application to fold recognition in genome **databases**.
AU Wallqvist A; Fukunishi Y; Murphy L R; Fadel A; Levy R M
CS Department of Chemistry, Rutgers University, Wright-Rieman Laboratories, 610 Taylor Rd, Piscataway, NJ 08854-8087, USA.. anders@rutchem.rutgers.edu
NC GM-30580 (NIGMS)
SO Bioinformatics (Oxford, England), (2000 Nov) 16 (11) 988-1002.

Journal code: 9808944. ISSN: 1367-4803.
CY England: United Kingdom
DT Journal; Article; (JOURNAL ARTICLE)
LA English
FS Priority Journals
EM 200104
ED Entered STN: 20010425
Last Updated on STN: 20010425
Entered Medline: 20010419

AB MOTIVATION: **Sequence** alignment techniques have been developed into extremely powerful tools for identifying the folding families and function of proteins in newly sequenced genomes. For a sufficiently low **sequence** identity it is necessary to incorporate additional structural information to positively detect homologous proteins. We have carried out an extensive analysis of the effectiveness of incorporating secondary structure information directly into the alignments for fold recognition and identification of distant protein homologs. A secondary structure similarity matrix based on a **database** of three-dimensionally aligned proteins was first constructed. An **iterative** application of dynamic programming was used which incorporates linear combinations of amino acid and secondary structure **sequence** similarity scores. Initially, only primary **sequence** information is used. Subsequently contributions from secondary structure are phased in and new homologous proteins are positively identified if their scores are consistent with the predetermined error rate. RESULTS: We used the SCOP40 **database**, where only PDB **sequences** that have 40% homology or less are included, to calibrate homology detection by the combined amino acid and secondary structure **sequence** alignments. Combining predicted secondary structure with **sequence** information results in a 8-15% increase in homology detection within SCOP40 relative to the pairwise alignments using only amino acid **sequence** data at an error rate of 0.01 errors per query; a 35% increase is observed when the actual secondary structure **sequences** are used. Incorporating predicted secondary structure information in the analysis of six small genomes yields an improvement in the homology detection of approximately 20% over SSEARCH pairwise alignments, but no improvement in the total number of homologs detected over PSI-BLAST, at an error rate of 0.01 errors per query. However, because the pairwise alignments based on combinations of amino acid and secondary structure similarity are different from those produced by PSI-BLAST and the error rates can be calibrated, it is possible to combine the results of both **searches**. An additional 25% relative improvement in the number of genes identified at an error rate of 0.01 is observed when the data is pooled in this way. Similarly for the SCOP40 dataset, PSI-BLAST detected 15% of all possible homologs, whereas the pooled results increased the total number of homologs detected to 19%. These results are compared with recent reports of homology detection using **sequence** profiling methods. AVAILABILITY: Secondary structure alignment homepage at http://lutece.rutgers.edu/ssas CONTACT: anders@rutchem.rutgers.edu; ronlevy@lutece.rutgers.edu Supplementary Information: Genome **sequence**/structure alignment results at http://lutece.rutgers.edu/ss_fold_predictions.

L10 ANSWER 17 OF 29 BIOSIS COPYRIGHT 2004 BIOLOGICAL ABSTRACTS INC. on STN Full Text
AN 2001:51030 BIOSIS
DN PREV200100051030
TI CAST: An **iterative** algorithm for the complexity analysis of **sequence** tracts.
AU Promponas, Vasilis J.; Enright, Anton J.; Tsoka, Sophia; Kreil, David P.; Leroy, Christophe; Hamodrakas, Stavros; Sander, Chris; Ouzounis, Christos

A. [Reprint author]
CS Computational Genomics Group, EMBL Cambridge Outstation, European Bioinformatics Institute, Cambridge, CB10 1SD, UK
SO Bioinformatics (Oxford), (October, 2000) Vol. 16, No. 10, pp. 915-922. print.
ISSN: 1367-4803.
DT Article
LA English
ED Entered STN: 24 Jan 2001
Last Updated on STN: 12 Feb 2002
AB Motivation: Sensitive detection and masking of low-complexity regions in protein **sequences**. Filtered **sequences** can be used in **sequence** comparison without the risk of matching compositionally biased regions. The main advantage of the method over similar approaches is the selective masking of single residue types without affecting other, possibly important, regions. Results: A novel algorithm for low-complexity region detection and selective masking. The algorithm is based on multiple-pass Smith-Waterman comparison of the query **sequence** against twenty homopolymers with infinite gap penalties. The output of the algorithm is both the masked query **sequence** for further analysis, e.g. **database searches**, as well as the regions of low complexity. The detection of low-complexity regions is highly specific for single residue types. It is shown that this approach is sufficient for masking **database** query **sequences** without generating false positives. The algorithm is benchmarked against widely available algorithms using the 210 genes of Plasmodium falciparum chromosome 2, a dataset known to contain a large number of low-complexity regions. Availability: CAST (version 1.0) executable binaries are available to academic users free of charge under license. Web site entry point, server and additional material: http://www.ebi.ac.uk/research/cgg/services/cast/. Contact: ouzounis@ebi.ac.uk.

L10 ANSWER 18 OF 29 MEDLINE on STN
Full Text
AN 2001092141 MEDLINE
DN PubMed ID: 11023840
TI Proteins of the endoplasmic-reticulum-associated degradation pathway: domain detection and function prediction.
AU Ponting C P
CS MRC Functional Genetics Unit, Department of Human Anatomy and Genetics, University of Oxford, South Parks Road, Oxford OX1 3QX, UK..
Chris.Ponting@anat.ox.ac.uk
SO Biochemical journal, (2000 Oct 15) 351 Pt 2 527-35.
Journal code: 2984726R. ISSN: 0264-6021.
CY ENGLAND: United Kingdom
DT Journal; Article; (JOURNAL ARTICLE)
LA English
FS Priority Journals
EM 200101
ED Entered STN: 20010322
Last Updated on STN: 20030215
Entered Medline: 20010125
AB **Sequence database searches**, using **iterative**-profile and Hidden-Markov-model approaches, were used to detect hitherto-undetected homologues of proteins that regulate the endoplasmic reticulum (ER)-associated degradation pathway. The translocon-associated subunit Sec63p (Sec=secretory) was shown to contain a domain of unknown function found twice in several Brr2p-like RNA helicases (Brr2=bad response to refrigeration 2). Additionally, Cue1p (Cue=coupling of ubiquitin conjugation to ER degradation), a yeast protein that recruits the

ubiquitin-conjugating (UBC) enzyme Ubc7p to an ER-associated complex, was found to be one of a large family of putative scaffolding-domain-containing proteins that include the autocrine motility factor receptor and fungal Vps9p (Vps=vacuolar protein sorting). Two other yeast translocon-associated molecules, Sec72p and Hrd3p (Hrd=3-hydroxy-3-methylglutaryl-CoA reductase degradation), were shown to contain multiple tetratricopeptide-repeat-like **sequences**. From this observation it is suggested that Sec72p associates with a heat-shock protein, Hsp70, in a manner analogous to that known for Hop (Hsp70/Hsp90 organizing protein). Finally, the luminal portion of Ire1p (Ire=high inositol-requiring), thought to convey the sensing function of this transmembrane kinase and endoribonuclease, was shown to contain repeats similar to those in beta-propeller proteins. This finding hints at the mechanism by which Ire1p may sense extended unfolded proteins at the expense of compact folded molecules.

L10 ANSWER 19 OF 29 MEDLINE on STN DUPLICATE 11
Full Text
AN 2000470784 MEDLINE
DN PubMed ID: 10842732
TI Fast assignment of protein structures to **sequences** using the intermediate **sequence** library PDB-ISL.
AU Teichmann S A; Chothia C; Church G M; Park J
CS MRC Laboratory of Molecular Biology, Cambridge, UK.. sat@mrc-lmb.cam.ac.uk
SO Bioinformatics (Oxford, England), (2000 Feb) 16 (2) 117-24.
Journal code: 9808944. ISSN: 1367-4803.
CY ENGLAND: United Kingdom
DT Journal; Article; (JOURNAL ARTICLE)
LA English
FS Priority Journals
EM 200010
ED Entered STN: 20001012
Last Updated on STN: 20001012
Entered Medline: 20001003
AB MOTIVATION: For large-scale structural assignment to **sequences**, as in computational structural genomics, a fast yet sensitive **sequence search** procedure is essential. A new approach using intermediate **sequences** was tested as a shortcut to **iterative** multiple **sequence search** methods such as PSI-BLAST. RESULTS: A library containing potential intermediate **sequences** for proteins of known structure (PDB-ISL) was constructed. The **sequences** in the library were collected from a large **sequence database** using the **sequences** of the domains of proteins of known structure as the query **sequences** and the **program** PSI-BLAST. **Sequences** of proteins of unknown structure can be matched to distantly related proteins of known structure by using pairwise **sequence** comparison methods to find homologues in PDB-ISL. **Searches** of PDB-ISL were calibrated, and the number of correct matches found at a given error rate was the same as that found by PSI-BLAST. The advantage of this library is that it uses pairwise **sequence** comparison methods, such as FASTA or BLAST2, and can, therefore, be searched easily and, in many cases, much more quickly than an **iterative** multiple **sequence** comparison method. The procedure is roughly 20 times faster than PSI-BLAST for small genomes and several hundred times for large genomes. AVAILABILITY: **Sequences** can be submitted to the PDB-ISL servers at http://stash.mrc-lmb.cam.ac.uk/PDB_ISL/ or http://cyrah.ebi.ac.uk:1111/Serv/PDB_ISL/ and can be downloaded from ftp://ftp.ebi.ac.uk/pub/contrib/jong/PDB_+_++ISL/ CONTACT: sat@mrc-lmb.cam.ac.uk and jong@ebi.ac.uk

L10 ANSWER 20 OF 29 MEDLINE on STN DUPLICATE 12
Full Text

AN 1999241053 MEDLINE
DN PubMed ID: 10222208
TI Gleaning non-trivial structural, functional and evolutionary information about proteins by **iterative database searches**.
AU Aravind L; Koonin E V
CS National Center for Biotechnology Information, National Library of Medicine, National Institutes of Health, Bethesda, MD 20894, USA.
SO Journal of molecular biology, (1999 Apr 16) 287 (5) 1023-40.
Journal code: 2985088R. ISSN: 0022-2836.
CY ENGLAND: United Kingdom
DT Journal; Article; (JOURNAL ARTICLE)
LA English
FS Priority Journals; Space Life Sciences
EM 199905
ED Entered STN: 19990601
Last Updated on STN: 19990601
Entered Medline: 19990519
AB Using a number of diverse protein families as test cases, we investigate the ability of the recently developed **iterative sequence database search** method, PSI-BLAST, to identify subtle relationships between proteins that originally have been deemed detectable only at the level of structure-structure comparison. We show that PSI-BLAST can detect many, though not all, of such relationships, but the success critically depends on the optimal choice of the query **sequence** used to initiate the **search**. Generally, there is a correlation between the diversity of the **sequences** detected in the first pass of **database** screening and the ability of a given query to detect subtle relationships in subsequent iterations. Accordingly, a thorough analysis of protein superfamilies at the **sequence** level is necessary in order to maximize the chances of gleaning non-trivial structural and functional inferences, as opposed to a single **search**, initiated, for example, with the **sequence** of a protein whose structure is available. This strategy is illustrated by several findings, each of which involves an unexpected structural prediction: (i) a number of previously undetected proteins with the HSP70-actin fold are identified, including a highly conserved and nearly ubiquitous family of metal-dependent proteases (typified by bacterial O-sialoglycoprotease) that represent an adaptation of this fold to a new type of enzymatic activity; (ii) we show that, contrary to the previous conclusions, ATP-dependent and NAD-dependent DNA ligases are confidently predicted to possess the same fold; (iii) the C-terminal domain of 3-phosphoglycerate dehydrogenase, which binds serine and is involved in allosteric regulation of the enzyme activity, is shown to typify a new superfamily of ligand-binding, regulatory domains found primarily in enzymes and regulators of amino acid and purine metabolism; (iv) the immunoglobulin-like DNA-binding domain previously identified in the structures of transcription factors NFkappaB and NFAT is shown to be a member of a distinct superfamily of intracellular and extracellular domains with the immunoglobulin fold; and (v) the Rag-2 subunit of the V-D-J recombinase is shown to contain a kelch-type beta-propeller domain which rules out its evolutionary relationship with bacterial transposases. Copyright 1999 Academic Press.

L10 ANSWER 21 OF 29 MEDLINE on STN
Full Text
AN 2001424384 MEDLINE
DN PubMed ID: 11471246
TI An evolutionary classification of the metallo-beta-lactamase fold proteins.
AU Aravind L
CS National Center for Biotechnology Information, National Library of

Medicine, National Institutes of Health, Bldg. 38A, Bethesda, MD 20894, USA.
SO In silico biology, (1999) 1 (2) 69-91.
Journal code: 9815902. ISSN: 1386-6338.
CY Netherlands
DT Journal; Article; (JOURNAL ARTICLE)
LA English
FS Priority Journals
EM 200108
ED Entered STN: 20010820
Last Updated on STN: 20010820
Entered Medline: 20010816
AB All the detectable metallo-beta-lactamase fold proteins were identified in the publicly available **sequence databases** and complete genome **sequences** using **iterative** profile **searches** with the PSI-BLAST **program** and motif **searches** with position specific weight matrices. The catalytic site/mechanism and the corresponding structural elements were characterized for these proteins based on the available structure of the Bacillus zinc-dependent beta-lactamase. Based on pair-wise **sequence** and phylogenetic analysis an evolutionary classification for enzymes of this fold was developed and discussed in terms of implications for substrate specificity. Finally, some predicted inactive members which have been recruited for non-enzymatic functions such as microtubule binding in a cytoskeletal MAP1 are described.

L10 ANSWER 22 OF 29 BIOSIS COPYRIGHT 2004 BIOLOGICAL ABSTRACTS INC. on STN
Full Text
AN 1998:442884 BIOSIS
DN PREV199800442884
TI An algorithm for the identification of proteins using peptides with ragged N- or C-terminal generated by **sequential** endo- and exopeptidase digestions.
AU Korostensky, Chantal; Staudenmann, Werner; Daninese, Paola; Hoving, Sjouke; Gonnet, Gaston; James, Peter [Reprint author]
CS Protein Chem. Lab., ETH-Zentrum, Universitaetsstr. 16, CH-8092 Zuerich, Switzerland
SO Electrophoresis, (Aug., 1998) Vol. 19, No. 11, pp. 1933-1940. print.
CODEN: ELCTDN. ISSN: 0173-0835.
DT Article
LA English
ED Entered STN: 21 Oct 1998
Last Updated on STN: 21 Oct 1998
AB We have developed an algorithm (MassDynSearch) for identifying proteins using a combination of peptide masses with small associated **sequences** (tags). Unlike the approach developed by Matthias Mann, 'Tag searching', in which the **sequence** tags are generated by gas phase fragmentation of peptides in a mass spectrometer, 'Rag Tag' searching uses peptide tags which are generated enzymatically or chemically. The protein is digested either chemically or with an endopeptidase and the resultant mixture is then subjected to partial exopeptidase degradation. The mixture is analyzed by matrix assisted laser desorption and ionization time of flight mass spectrometry and a list of intact peptide masses is generated, each associated with a set of degradation product masses which serve as unique tags. These 'tagged masses' are used as the input to an algorithm we have written, MassDynSearch, which **searches** protein and DNA **databases** for proteins which contain similar tagged motifs. The method is simple, rapid and can be fully automated. The main advantage of this approach is that the specificity of the initial digestion is unimportant since multiple peptides with tags are used to **search** the **database**. This is especially useful for proteins like membrane, cytoskeletal, and other

proteins where specific endopeptidases are less efficient and lower specificity proteases such as chymotrypsin, pepsin, and elastase must be used.

L10 ANSWER 23 OF 29 MEDLINE on STN DUPLICATE 13
Full Text
AN 1998095714 MEDLINE
DN PubMed ID: 9434271
TI Evolutionary relationships among proteins probed by an **iterative** neighborhood cluster analysis (INCA). Alignment of bacteriorhodopsins with the yeast **sequence** YRO2.
AU Graul R C; Sadee W
CS Department of Biopharmaceutical Sciences, University of California San Francisco 94143-0446, USA.
NC DA04166 (NIDA)
GM37188 (NIGMS)
GM43102 (NIGMS)
SO Pharmaceutical research, (1997 Nov) 14 (11) 1533-41.
Journal code: 8406521. ISSN: 0724-8741.
CY United States
DT Journal; Article; (JOURNAL ARTICLE)
LA English
FS Priority Journals
EM 199802
ED Entered STN: 19980226
Last Updated on STN: 19980226
Entered Medline: 19980219
AB PURPOSE: Searching the existing **databases** for homologous **sequences** is essential to understanding a protein's structure and function. For a query **sequence**, its nearest neighbors can be identified by BLAST (basic local alignment **search** tool). However, a single query **sequence** is sufficient to define the entire neighborhood of related **sequences**, and multiple BLAST queries are needed. We describe here a **program** which permits automated and **iterative** BLAST analysis of an entire neighborhood of **sequences** and apply this to **search** for homologs of the bacteriorhodopsins outside the archaea phylum. METHODS: We have developed a Java **program**, '**Iterative** Neighborhood Cluster Analysis' (INCA), which performs **iterative** BLAST **searches**, beginning with a single starter **sequence**, and proceeding with any other **sequence** achieving a predefined minimum alignment score. This results in a cluster of **sequences** where each **sequence** is related to at least one other **sequence** by the cutoff score, additional lists of more distantly related **sequences** for each member of cluster. RESULTS: Bacteriorhodopsins had not been previously aligned with any other protein family with scores indicative of probable homology. Using INCA, we identified a probable homolog in yeast, YRO2_YEAST, also containing seven putative transmembrane domains. A finding of probable homology was supported by additional alignment strategies. CONCLUSIONS: INCA is a useful tool to assess complete protein neighborhoods. With an increasing **database**, INCA can serve to detect the emergence of evolutionary links between even the most distantly related protein families. Identifying a homolog of the bacteriorhodopsins in yeast illustrates this approach but at the same time highlights the vast evolutionary distances between polytopic membrane proteins, such as the bacteriorhodopsins.

L10 ANSWER 24 OF 29 MEDLINE on STN
Full Text
AN 96338748 MEDLINE
DN PubMed ID: 8743692
TI **Iterative** template refinement: protein-fold prediction using **iterative**

search and hybrid **sequence**/structure templates.
AU Yi T M; Lander E S
CS Whitehead Institute for Biomedical Research, Massachusetts Institute of Technology, Cambridge 02142, USA.
SO Methods in enzymology, (1996) 266 322-39.
Journal code: 0212271. ISSN: 0076-6879.
CY United States
DT Journal; Article; (JOURNAL ARTICLE)
LA English
FS Priority Journals
EM 199610
ED Entered STN: 19961022
Last Updated on STN: 19961022
Entered Medline: 19961010

L10 ANSWER 25 OF 29 MEDLINE on STN
Full Text
AN 97136696 MEDLINE
DN PubMed ID: 8982073
TI Cloning and **sequence** analysis of the candidate nicotinic acetylcholine receptor alpha subunit gene tar-1 from Trichostrongylus colubriformis.
AU Wiley L J; Weiss A S; Sangster N C; Li Q
CS Department of Veterinary Pathology, University of Sydney, N.S.W, Australia.
SO Gene, (1996 Dec 5) 182 (1-2) 97-100.
Journal code: 7706761. ISSN: 0378-1119.
CY Netherlands
DT Journal; Article; (JOURNAL ARTICLE)
LA English
FS Priority Journals
OS GENBANK-U56903
EM 199701
ED Entered STN: 19970219
Last Updated on STN: 19980206
Entered Medline: 19970122
AB A T. colubriformis genomic library in lambda EMBL3 was screened for **sequences** homologous to the Caenorhabditis elegans unc-38 nicotinic acetylcholine receptor (nAChR) alpha-subunit gene. The candidate gene tar-1 (for Trichostrongylus acetylcholine receptor subunit gene 1) comprising 13704 base pairs was thus identified. BLAST comparison of the sequenced clone with GenBank, followed by comparison of translated regions in six reading frames with protein **databases**, identified clearly defined tracts corresponding to 12 putative exons sharing high **sequence** homology to other nAChR genes and able to code for **sequential** regions of a putative nAChR alpha-subunit protein (tar-1). Tar-1 shares **sequence** similarities with over 40 nAChR subunit proteins. The highest similarity (91.6%) is with unc-38, suggesting that nAChR **sequences** from nematodes are closely related. The **sequence** includes motifs typical of these molecules including adjacent cysteine residues at the ACh binding site and four transmembrane regions. The DNA **sequence** presents the longest genomic tract described for this organism and should prove useful as a probe source in the **search** for nAChR genes from this and other nematodes and for studying the molecular mechanism of resistance to levamisole, a drug which is known to act on nAChRs of worms and which is widely used for parasite control.

L10 ANSWER 26 OF 29 MEDLINE on STN DUPLICATE 14
Full Text
AN 96348763 MEDLINE
DN PubMed ID: 8744771

TI XFINGER: a tool for searching and visualising protein fingerprints and patterns.
AU Perkins D N; Attwood T K
CS Department of Biochemistry, University of Leeds, UK.
SO Computer applications in the biosciences : CABIOS, (1996 Apr) 12 (2) 89-94.
Journal code: 8511758. ISSN: 0266-7061.
CY ENGLAND: United Kingdom
DT Journal; Article; (JOURNAL ARTICLE)
LA English
FS Priority Journals
EM 199611
ED Entered STN: 19961219
Last Updated on STN: 20000303
Entered Medline: 19961106
AB A tool for searching pattern and fingerprint **databases** is described. Fingerprints are groups of motifs excised from conserved regions of **sequence** alignments and used for **iterative database** scanning. The constituent motifs are thus encoded as small alignments in which **sequence** information is maximised with each **database** pass; they therefore differ from regular-expression patterns, in which alignments are reduced to single consensus **sequences**. Different **database** formats have evolved to store these disparate types of information, namely the PROSITE dictionary of patterns and the PRINTS fingerprint **database**, but **programs** have not been available with the flexibility to **search** them both. We have developed a facility to do this: the system allows query **sequences** to be scanned against either PROSITE, the full PRINTS **database**, or against individual fingerprints. The results of fingerprint **searches** are displayed simultaneously in both text and graphical windows to render them more tangible to the user. Where structural coordinates are available, identified motifs may be visualised in a 3D context. The **program** runs on Silicon Graphics machines using GL graphics libraries and on machines with X servers supporting the PEX extension: its use is illustrated here by depicting the location of low-density lipoprotein-binding (LDL) motifs and leucine-rich repeats in a mosaic G-protein-coupled receptor (GPCR).

L10 ANSWER 27 OF 29 MEDLINE on STN DUPLICATE 15
Full Text
AN 95379079 MEDLINE
DN PubMed ID: 7650738
TI A **sequence** property approach to searching protein **databases**.
AU Hobohm U; Sander C
CS EMBL-European Molecular Biology Laboratory, Heidelberg, Germany.
SO Journal of molecular biology, (1995 Aug 18) 251 (3) 390-9.
Journal code: 2985088R. ISSN: 0022-2836.
CY ENGLAND: United Kingdom
DT Journal; Article; (JOURNAL ARTICLE)
LA English
FS Priority Journals
EM 199509
ED Entered STN: 19951005
Last Updated on STN: 19951005
Entered Medline: 19950928
AB Currently available **sequence** alignment **programs** are generally not capable of detecting functional and structural homologs in the twilight zone of **sequence** similarity, i.e. when the **sequence** identity falls below about 25%. Here we attempt to detect such weak similarities using an approach based on a notion of protein **sequence** similarity radically different from that used in **sequential** alignment. The approach defines

protein **sequence** dissimilarity (or distance) as a weighted sum of differences of compositional properties such as singlet and doublet amino acid composition, molecular weight, isoelectric point (protein property **search** or PropSearch). With PropSearch, either single **sequences** can be used for a **database** query, or multiple **sequences** can be merged into an "average" **sequence** reflecting the average composition of a protein family. First, we show that members of structural protein families have a low mutual PropSearch distance when the weights are optimized to discriminate maximally between structural families. Second, we demonstrate the results of **database searches** using the PropSearch method. Such **searches** are very rapid when scanning a preprocessed **database** and do not require alignments. In cases in which conventional alignment tools fail to detect similarities, PropSearch can be used to generate hypotheses about possible structural or functional relationships between a new **sequence** and **sequences** in the **database**.

L10 ANSWER 28 OF 29 MEDLINE on STN DUPLICATE 16
Full Text
AN 95078739 MEDLINE
DN PubMed ID: 7987226
TI Recognition of related proteins by **iterative** template refinement (ITR).
AU Yi T M; Lander E S
CS Whitehead Institute for Biomedical Research, Massachusetts Institute of Technology, Cambridge 02142.
SO Protein science : a publication of the Protein Society, (1994 Aug) 3 (8) 1315-28.
Journal code: 9211750. ISSN: 0961-8368.
CY United States
DT Journal; Article; (JOURNAL ARTICLE)
LA English
FS Priority Journals
EM 199501
ED Entered STN: 19950124
Last Updated on STN: 19950124
Entered Medline: 19950111
AB Predicting the structural fold of a protein is an important and challenging problem. Available computer **programs** for determining whether a protein **sequence** is compatible with a known 3-dimensional structure fall into 2 categories: (1) structure-based methods, in which structural features such as local conformation and solvent accessibility are encoded in a template, and (2) **sequence**-based methods, in which aligned **sequences** of a set of related proteins are encoded in a template. In both cases, the **programs** use a static template based on a predetermined set of proteins. Here, we describe a computer-based method, called **iterative** template refinement (ITR), that uses templates combining structure-based and **sequence**-based information and employs an **iterative search** procedure to detect related proteins and sequentially add them to the templates. Starting from a single protein of known structure, ITR performs **sequential** cycles of **database search** to construct an expanding tree of templates with the aim of identifying subtle relationships among proteins. Evaluating the performance of ITR on 6 proteins, we found that the method automatically identified a variety of subtle structural similarities to other proteins. For example, the method identified structural similarity between arabinose-binding protein and phosphofructokinase, a relationship that has not been widely recognized.

L10 ANSWER 29 OF 29 MEDLINE on STN DUPLICATE 17
Full Text
AN 91243391 MEDLINE
DN PubMed ID: 2036781

TI A parallel computing approach to genetic **sequence** comparison: the master-worker paradigm with interworker communication.
AU Sittig D F; Foulser D; Carriero N; McCorkle G; Miller P L
CS Department of Anesthesiology, Yale University, New Haven, Connecticut 06510.
NC RO1 LM05044 (NLM)
SO Computers and biomedical research, an international journal, (1991 Apr) 24 (2) 152-69.
Journal code: 0100331. ISSN: 0010-4809.
CY United States
DT Journal; Article; (JOURNAL ARTICLE)
LA English
FS Priority Journals
EM 199106
ED Entered STN: 19910719
Last Updated on STN: 19910719
Entered Medline: 19910628
AB We have implemented a parallel version of a dynamic programming biological **sequence** comparison algorithm to study the potential applicability of using parallel computers for genetic **sequence** comparisons. Our parallel **program** is built using C-Linda, a machine-independent parallel programming language, and was tested on both a 10 CPU Sequent Symmetry and a 64 CPU Intel Hypercube. C-Linda implements a shared associative memory model, "tuple space," through which multiple processes can communicate and coordinate control. In our master-worker (MW) parallel implementation, a master process creates several worker processes, extracts a test **sequence** and multiple library **sequences** from a **database** and stores them in tuple space. Each worker reads the test **sequence** and then repeatedly extracts library strings from tuple space, performs pairwise **sequence** comparison using a local comparison algorithm to generate a similarity score, and returns the similarity scores to tuple space. The master collects the scores from tuple space and identifies the best match over all library **sequences**. We also implemented a method of global interworker communication to reduce the total **search** time by stopping those string comparisons that had no chance of improving on the current best match. Comparisons of the total run time, speedup, and efficiency were made for parallel and **sequential** versions of a basic MW implementation as well as versions with the global abort threshold.

```
=> d his

     (FILE 'HOME' ENTERED AT 15:39:31 ON 20 AUG 2004)

     FILE 'MEDLINE, BIOSIS' ENTERED AT 15:39:40 ON 20 AUG 2004
                E TOLDO L/AU
L1           21 S E3-6
L2           18 DUPLICATE REMOVE L1 (3 DUPLICATES REMOVED)
                E RIPPMANN F/AU
L3           32 S E15-16
L4           25 DUPLICATE REMOVE L3 (7 DUPLICATES REMOVED)
L5          394 S SEQUENCE AND SEARCH AND (ITERATIVE OR SEQUENTIAL)
L6          150 S L5 AND DATABASE
L7            6 S L6 AND (REMOV? OR SEPARAT?)
L8            5 DUPLICATE REMOVE L7 (1 DUPLICATE REMOVED)
L9           46 S L6 AND (SOFTWARE OR PROGRAM)
L10          29 DUPLICATE REMOVE L9 (17 DUPLICATES REMOVED)

=> s 16 and prun?
L11           0 L6 AND PRUN?
```

```
=> log y
COST IN U.S. DOLLARS                        SINCE FILE      TOTAL
                                              ENTRY      SESSION
FULL ESTIMATED COST                           74.64        74.85

STN INTERNATIONAL LOGOFF AT 16:02:14 ON 20 AUG 2004
```